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**Optimal Pulsed Pumping Schedule Using  
Calculus of Variation Methodology**

**Thesis**

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**AFIT/GEE/ENC/99M-1.**

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Variation Methodology***

**Thesis**

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Master of Science in Engineering and Environmental Management

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USING CALCULUS OF VARIATION METHODOLOGY

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## *List of Symbols*

### English Symbols

Symbol	Description
$B$	aquifer thickness
$c$	contaminant concentration
$c_s$	concentration standard
$D$	hydrodynamic dispersion tensor
$D^*$	molecular diffusion coefficient
$G$	optimization function
$h$	hydraulic head
$K$	hydraulic conductivity
$K_d$	distribution coefficient
$\mathcal{L}$	Lagrangian
$m$	regional hydraulic gradient
$s$	sorbed concentration
$T$	transmissivity
$\mathbf{v}$	fluid velocity vector
$z$	weighting factor

### Greek Symbols

Symbol	Description
--------	-------------

$\alpha_L$	longitudinal dispersivity
$\alpha_T$	transverse dispersivity
$\theta$	porosity
$\xi$	essential concentration function
$\rho_w$	water density
$\rho_B$	bulk density
$\sigma$	concentration scaling factor

### Abbreviations/Acronyms

Abbreviation	Description
AFCEE	Air Force Center for Environmental Excellence
AFIT	Air Force Institute of Technology
AU	Air University
EPA	Environmental Protection Agency
GMS	Groundwater Modeling System
LEA	Local Equilibrium Assumptions
MODFLOW	Numerical Three-Dimensional Finite-Differences Flow Code
MT3D	Numerical Three-Dimensional Transport Code
USGS	United States Geological Survey
WES	Waterways Experiment Station, U.S. Army Corps of Engineers
WHO	World Health Organization

## *Abstract*

Application of a variational optimization technique has demonstrated the potential strength of pulsed pumping operations for use at existing pump-and-treat aquifer remediation sites. The optimized pulsed pumping technique has exhibited notable improvements in operational effectiveness over continuous pumping. The optimized pulsed pumping technique has also exhibited an advantage over uniform time intervals for pumping and resting cycles. The most important finding supports the potential for managing and improving pumping operations in the absence of complete knowledge of plume characteristics. An objective functional was selected to minimize mass of water removed and minimize the non-essential mass of contaminant removed. General forms of the essential concentration function were analyzed to determine the appropriate form required for compliance with management preferences. Third-order essential concentration functions provided optimal solutions for the objective functional. The results of using this form of the essential concentration function in the methodology provided optimal solutions for the switching times. The methodology was applied to a hypothetical, two-dimensional aquifer influenced by specified and no-flow boundaries, injection wells and extraction wells. Flow simulations used MODFLOW, transport simulations used MT3D, and the graphical interface for obtaining concentration time series data and flow/transport links were generated by GMS version 2.1.

# *Optimal Pulsed Pumping Schedule Using Calculus of Variation Methodology*

## **I. Introduction**

### **I.1 Background**

Clean, high-quality water, suitable for consumption, is a natural resource we often take for granted. In the United States accessibility is generally universal, and only occasionally becomes a concern such as during natural disasters. Even then the temporary situation is usually corrected within a matter of days. To support the demand for potable water, people look to practically ubiquitous geological sources known as aquifers to yield their groundwater reserves. Groundwater is the source of about one-third of this country's drinking water and, excluding water for power plant cooling, it supplies almost 40 percent of our total water withdrawals [36]. Rural areas almost exclusively rely on groundwater and many of the largest cities require groundwater to satisfy their demands. Unfortunately, past mistakes of ignorance have created problems of contamination, which hinder the current use of groundwater as a drinking water source. The National Research Council estimates that there are between 300,000 and 400,000 sites in the United States that may have contaminated soil or groundwater requiring some form of remediation [39]. The serious nature of groundwater contamination is complicated by two main problems. First, contamination presents a long-term problem. Buried wastes are a typical source of contamination and have usually been buried for several decades. These buried wastes are not well documented or

have been forgotten entirely, and it takes many years for any indication of a release to manifest itself. By the time of discovery, the contamination has usually migrated considerable distances. The second complication is in restoring groundwater to its original state once it has been contaminated. Experience does not strongly support this even as a possibility, and the problem of cleanup translates into enormous costs. For example, relatively simple remediation sites involve the removal of an underground storage tank. These operations average about \$100,000 each, but more complicated sites cost an average of \$27 million each [52]. Clearly these costs will reach into many billions of dollars. The imperative to make smart remediation choices is upon us to not waste any money or resources on ineffective methods and technologies.

## **I.2 General Issue**

Long term operations of in-place environmental remediation systems will carry the bulk of total Air Force environmental investments in the future. For the Air Force Base Conversion Agency (AFBCA) alone, the total long term operation will top \$1.1 billion through year 2005 [58]. Active USAF installations will also invest large proportions of funding in the coming years. In light of the heavy investment, new ways of regarding the cost effectiveness must be developed to lead to better management decisions.

Many groundwater remediation projects incorporate pump-and-treat technology with the objective of restoring an aquifer. Approximately three-quarters of all groundwater remediation projects use pump-and-treat technology with an estimate of 3000 sites in operation in the United States [36]. Pump-and-treat systems have unfortunately displayed severe limitations with regard to remediation. First, the presence of non-aqueous phase liquids

(NAPL) complicates or even frustrates the removal of contamination by pump-and-treat systems alone. NAPLs are a pure phase, low solubility liquid and should not be expected to go into solution easily. In addition, many NAPLs are denser than water, and therefore tend to sink below the water table to depths that are very difficult to reach or even locate. Another limitation is seen at the field-scale where diffusion into and out of tight formations like clay layers exhibits rate-limited sorption behavior. The behavior is observed when contaminant concentrations decrease over time and asymptotically approach a residual level [31]. This response is typically called tailing. In some cases, as the contaminants desorb into the aquifer, the concentration levels actually increase, or rebound, after pumping has stopped [35]. This sorption/desorption process illustrates the concept of rate-limited sorption. Often the sorbed contaminant mass is much greater than the dissolved mass [9], [35].

Tailing and rebound occur as a result of several different phenomena that are usually present in aquifer systems such as dissolution, diffusion, and desorption [53]. Determination of sorption and desorption rates require careful consideration of site conditions, over and above the basic concentration-versus-time aspect. With the assistance of analytical and numerical models, rate-limited sorption/desorption profoundly effects the transport of sorbing organic contaminants [24], [41], [54]. Rate-limited sorption is due to the slow diffusion of contaminant from essentially immobile regions to more mobile regions. Given a general aquifer system, Goltz and Oxley demonstrated in their work the vital necessity of rate-limited sorption and transport considerations when estimating aquifer cleanup time [23].

The presence of NAPL and rate-limited sorption characteristics are common limitations. The National Research Council evaluated 77 sites where pump-and-treat systems were operating and found only two sites where goals were likely to be achieved within a reasonable time and cost [39]. In contrast, 42 sites were considered extremely hard or impossible to cleanup due to NAPL and complex hydrogeology (sorption and heterogeneity). Apparently the goal of complete remediation seems futile for most pump-and-treat sites, thus the remediation manager must incorporate other remediation technologies and strategies into the existing pump and treat system to arrive at a better solution for the remediation question.

Pulsed pumping, a pumping schedule with alternate pumping and resting time intervals, has been suggested as a means to address tailing, flush stagnation zones by selective well cycling, and increase pump-and-treat effectiveness [8], [26], [31]. During the resting time interval, slower moving groundwater allows dissolved contamination concentrations to increase due to greater contributions by diffusion and desorption. During the active (pumping) time interval, higher concentrations are removed, thus increasing the rate of contaminant removal for that time interval. Contaminant concentrations will decline rapidly until the next resting interval resumes. The potential to significantly reduce pump operation costs, reduce groundwater extraction, and improve contaminant removal efficiencies exists.

### **I.3 Research Problem**

The general goal of this work is to produce a simulation tool that will aid the remediation manager with improving the effectiveness of an existing pump-and-treat system. The

long range perspective of this work targets the problems of rate-limited sorption, NAPLs, and contaminants in low conductivity regions. In these cases, conventional pump-and-treat technology has fallen short of expectations as a viable remediation technique and is acceptable only for perpetual hydraulic gradient control. Many emerging remediation technologies, which potentially could be very effective, are still in the development stage. Other technologies, more effective than pump-and-treat, may be unavailable or unsuitable for a given situation. Given these considerations, the focus of this work is the development of an optimization technique for pulsed pumping operations to improve existing pump-and-treat systems in the interim.

This thesis develops a mathematical tool combining contaminant transport with variational optimization techniques for use at existing, pump-and-treat remediation systems. Typically, pulsed pumping schedules are determined through trial-and-error methods. This work proposes a mathematical optimization of the pulsed pumping schedule with the constraints of contamination containment and well water drawdown. The application is meant for the immediate short term problem. The long term problem looks for a new technology to emerge and replace or augment existing pump-and-treat remediation to establish new shorter timelines for restoration. The solution to the long term problem is outside the scope of this work. Until such time when an effective long term solution emerges, optimal pulsed pumping remediation will reduce project costs over a presumably (but hopefully not) indefinite period.

The specific objectives of this research are:

1. Develop the consideration and selection of the essential concentration function, and

highlight the effect the form has on the objective function.

2. Clarify and expand the results used in an example to demonstrate the concept.
3. Determine the optimal pulsed pumping schedule for the objective function associated with the essential concentration function.
4. Considering the demonstration example, compare the optimization methodology performance with continuous pumping methodologies.

## **I.4 Aquifer Viewpoint**

The aquifer viewpoint is based on the concept of confined and unconfined aquifers. In this work, the focus is on the former where the top is bounded by a confining bed and the lower boundary is impermeable bedrock. The analysis of this aquifer is therefore does not contain the complexity of vertical flow components. This is done to isolate effects of methodology development. The next step is to establish governing equations that will be used to derive and develop the optimization methodology.

### **I.4.1 Aquifer Concepts**

One of the most important parameters in modeling an aquifer is hydraulic conductivity. Darcy developed hydraulic conductivity as a coefficient of proportionality describing the rate at which water can move through a porous medium [16]. The density and kinematic viscosity of the water must be considered in determining hydraulic conductivity. Both are functions of temperature, and therefore both will vary with the temperature of the water. Salinity also has an impact of water density and viscosity and is a major consideration in establishing initial conditions of the aquifer. Another parameter, related to hydraulic

conductivity, is the intrinsic permeability. As shown in Table 1, intrinsic permeability and hydraulic conductivity have a wide-range of values for unconsolidated sediments[16].

A concept that is also derived from hydraulic conductivity may be helpful in describing aquifer characteristics. Transmissivity is a measure of the amount of water that can be transmitted horizontally through a unit width by the full saturated thickness of the aquifer under a hydraulic gradient of 1. Transmissivity is the product of the hydraulic conductivity and the saturated thickness of the aquifer.

When the hydraulic head in a saturated aquifer changes, water will be either stored or released as a result of compression of the aquifer material and pore water. The storativity is the volume of water that a permeable unit will absorb or release from storage per unit surface area per unit change in head. Specific storage is the amount of water per unit volume of a saturated formation that is stored or released per unit change in head.

On a larger scale, aquifers are generally described as being either homogeneous or heterogeneous. Homogeneous implies that aquifer properties are uniform throughout the domain of interest. A relatively small scale is required for observations of variability. Heterogeneous implies a high level of spatial variability. The variability may be from changes in material or structure. Even with constant material and structure, an aquifer may still be considered heterogeneous due to large-scale dimensional changes such as a formation that

Material	Intr. Permeability (darcys)	Hydraulic Conductivity (cm/s)
Clay	$10^{-6}$ - $10^{-3}$	$10^{-9}$ - $10^{-6}$
Silt, sandy silts, clayey sands, till	$10^{-3}$ - $10^{-1}$	$10^{-6}$ - $10^{-4}$
Silty sands, fine sands	$10^{-2}$ - 1	$10^{-5}$ - $10^{-3}$
Well-sorted sands, glacial outwash	$1-10^2$	$10^{-3}$ - $10^{-1}$
Well-sorted gravel	$10-10^3$	$10^{-2}$ - 1

Table . 1. Ranges of Hydraulic Conductivity

gets thicker or thinner. Layering within an aquifer can produce heterogeneity, even if each layer is completely uniform within itself, because of differing hydraulic properties within each layer.

Isotropy or anisotropy is usually considered concurrently with homogeneity. Within the porous media, if the geometry of the voids is basically the same in all directions, then the hydraulic conductivity is uniform in all directions and there is isotropy. If, however, the geometry of the voids is not uniform, then hydraulic conductivity is probably greater in a certain direction, and the aquifer is considered anisotropic.

#### **I.4.2 Governing Equations**

The following assumptions were used as a basis for the methodology in this work:

1. A single extraction well was assumed to create one of two influences on a theoretical aquifer with a contaminant plume. A regional hydraulic gradient provides the other influence.
2. The confined aquifer and contaminated region were assumed to have a general rectangular geometry in two and three dimensions, and the media was assumed homogeneous and isotropic. Also, initial and boundary conditions show this general geometry.
3. No external contaminant sources or sinks were present, therefore a measurable initial concentration was assumed.
4. A piecewise constant, pulsed pumping schedule was assumed on the time interval,  $[0, t_f]$ , that allowed for  $n$  on/off intervals of varying length.

5. Rate-limited sorption/desorption is represented with a linear rate equation [23], [54].

The equations for advective-dispersive contaminant transport, coupled with the first-order rate expression are written as

$$\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D} \nabla c) - \nabla \cdot (\mathbf{v} c) - \frac{\rho_B}{\theta} \frac{\partial s}{\partial t} \quad (1)$$

and

$$\frac{\partial s}{\partial t} = \alpha (K_d c - s), \quad (2)$$

where  $c(x, t)$  is the contaminant concentration of the water phase [M/L<sup>3</sup>],  $s(x, t)$ , is the sorbed contaminant concentration [dimensionless],  $x$  is a rectangular coordinate point [L],  $t$  is time [T],  $\rho_B$  is the bulk density [M/L<sup>3</sup>],  $\theta$  is the porosity of the aquifer [dimensionless],  $\alpha$  is a linear rate constant [1/T],  $K_d$  is a distribution coefficient [L<sup>3</sup>/M],  $\mathbf{D}$  is the hydrodynamic dispersion tensor [L<sup>2</sup>/T], given for isotropic media in two dimensions as

$$\mathbf{D} = \begin{bmatrix} \alpha_L |\mathbf{v}| + D^* & 0 \\ 0 & \alpha_T |\mathbf{v}| + D^* \end{bmatrix} \quad (3)$$

and in three dimensions as

$$\mathbf{D} = \begin{bmatrix} \alpha_L |\mathbf{v}| + D^* & 0 & 0 \\ 0 & \alpha_T |\mathbf{v}| + D^* & 0 \\ 0 & 0 & \alpha_T |\mathbf{v}| + D^* \end{bmatrix} \quad (4)$$

where  $\alpha_L$  and  $\alpha_T$  are the longitudinal and transverse dispersivities of the porous media respectively [L],  $D^*$  is the molecular diffusion coefficient [L<sup>2</sup>/T], and  $|\mathbf{v}|$  is the magnitude of the velocity vector  $\mathbf{v}$  [L/T], determined by the head equation given as

$$\mathbf{v} = -\frac{1}{\theta} \mathbf{K} \nabla h \quad (5)$$

where  $\mathbf{K}$  is the hydraulic conductivity tensor of the porous media [L/T] and  $h$  is the hydraulic head [L].

The coupled equations, (1) and (2), describe the contaminant transport process and provide the partial differential equations for the boundary-value problem (BVP) which constrains the objective functional of the optimization problem. The boundary conditions for the BVP are

$$(\mathbf{D}\nabla c) \cdot \hat{\mathbf{n}} = 0 \quad (6)$$

at the well, for all time  $t > 0$ , where concentration in the well does not change due to hydrodynamic dispersion and

$$(\mathbf{v}c - \mathbf{D}\nabla c) \cdot \hat{\mathbf{n}} = 0 \quad (7)$$

where zero flux conditions exist at the boundary of the aquifer for all time  $t > 0$ . The  $\hat{\mathbf{n}}$  represents the physical dimensions in general form. Finally the initial conditions are expressed as

$$c(\mathbf{x}, 0) = c_0(\mathbf{x}) \quad (8)$$

for  $\mathbf{x}$  in the aquifer, and

$$s(\mathbf{x}, 0) = s_0(\mathbf{x}) \quad (9)$$

where  $c_0$  and  $s_0$  are the initial contaminant concentrations at time zero in the aqueous and solid phases at any point  $\mathbf{x}$  throughout the domain of the aquifer.

In the statement of the optimization problem, the transport equations stated in (1) and (2) will be treated as finite subsidiary conditions (constraints) imposed on the admissible functions for which the stated objective functional has an extremum. Therefore, the constraints are not as awkward when combined into a single equation. Thus, introducing the integrating factor  $e^{\alpha t}$  into equation (2), an expression for the sorbed concentration is found

as

$$s(\mathbf{x}, t) = e^{-\alpha t} s_0(\mathbf{x}) + \alpha K_d e^{-\alpha t} \int_0^t c(\mathbf{x}, \tau) e^{\alpha \tau} d\tau. \quad (10)$$

Combining equations (1), (2), and (10) and denoting the partial derivative of the concentration with respect to time as a subscript  $t$  (i.e.  $c_t = \frac{\partial c}{\partial t}$ ), then

$$\nabla(\mathbf{D} \nabla c) - \nabla \cdot (\mathbf{v} c) - \frac{\rho_B \alpha K_d}{\theta} c + \frac{\rho_B \alpha}{\theta} e^{-\alpha t} s_0(\mathbf{x}) + \frac{\rho_B \alpha^2 K_d}{\theta} \int_0^t e^{\alpha(\tau-t)} c(\mathbf{x}, \tau) d\tau - c_t = 0. \quad (11)$$

## I.5 Scope and Limitations of Research

This research develops an application of optimal pulsed pumping methodology built to solve the optimization problem using a calculus of variation approach. The Lagrange multiplier theory is instrumental in establishing an objective function and constraints that are intrinsic to optimization problem. An aquifer model provides a test bed for the methodology and a source for collecting data.

Limitations in this research primarily associated with the numerical simulation error when numerical approximations are made to calculate flow and transport solutions. The hypothetical aquifer model is characterized by a single extraction well, a single monitoring point, and constant head and no-flow boundaries. Plume concentration and dimensions are governed by a single injection period and transient hydraulic gradients influenced by a uniform regional gradients and well operations. The simulated aquifer is confined, unitary, and slightly heterogeneous and anisotropic. The simulation lacks rate-limited sorption characteristics, thus tailing and rebound are a result of macro-scale properties.

The methodology makes numerical approximations with regard to the first and second time derivatives of the concentration. Also, a simplifying assumption was made about the relationship between the derivatives before and after switching times.

## I.6 Overview

This thesis is divided into five chapters. Chapter 1 provides the general conditions surrounding the remediation problem and a roadmap to follow this work. Chapter 2 contains a review of literature sources that contribute to the theoretical basis of this thesis and justifications for pursuing this problem. Chapter 3 develops the optimization methodology relevant to this work and establishes a foundation for gathering data. The settings and inputs necessary for the simulations to run are also included in Chapter 3. Chapter 4 applies the methodology presented in Chapter 3 and presents graphical and tabular results of the simulation outcomes. Chapter 5 will summarize the research and develop conclusions from the findings. Limitations and further research recommendations are also stated in Chapter 5.

## II. Literature Review

This chapter reviews current research on pump-and-treat technology and optimization through model development and analysis. The principles of calculus of variations are employed to optimize a pulsed pumping schedule while ensuring containment for an existing remediation system.

### II.1 Pump-and-Treat Methods

About three-quarters of all groundwater remediation sites use pump-and-treat technology. Yet, rarely are cleanup goals met and the time needed to reach health-based requirements for groundwater quality is often underestimated [39]. Several research efforts are attempting to address problems associated with the lengthy process of meeting cleanup objectives [28], [33], [46]. Many remediation sites incorporate conventional pump-and-treat methods, but such systems often are not appropriate due largely to hydrological and contaminant-related limitations [53].

Many factors contribute to lengthy cleanup times encountered by pump-and-treat systems, but the primary hindrance can be attributed to the presence of contaminant in soil regions, which are not very accessible [43]. If the contaminant has sorbed to the soil or is located in a clay layer, it is in a region which is basically immobile. If the mass transfer of the contaminant is rate-limited, the problem of immobility is compounded.

Another reason for unexpected increases in cleanup times is that initial estimates often use analytical or numerical models based on instantaneous equilibrium assumptions between the aqueous and sorbed contaminant. Also known as the local equilibrium assumption (LEA), sorbed contaminant desorbs instantaneously into clean water as contaminated

water is removed by pumping. Depending on the soil and contaminant characteristics, the LEA could be completely invalid. This would result in a gross underestimation of cleanup times. Tailing and rebound are also attributed, in part, to mass transfer limitations such as rate-limited sorption [35].

## **II.2 Capture Zone Analysis**

Important concomitants of the pump-and-treat design are the determinations of containment, restoration area, and volume. Once these determinations are made, the pump-and-treat design requires capture zone analysis for the assessment of a performance monitoring plan based on the predicted flow field [53].

The capture zone of the aquifer due to the extraction well should not be confused with the drawdown radius of influence. The radius of influence is primarily determined from the transmissivity and pumping rate under steady-state conditions. The capture zone depends upon the regional hydraulic gradient as well as the transmissivity and pumping rate. Capture zones become narrower as the hydraulic gradient increases, and coincide with the radius of influence as the hydraulic gradient approaches zero.

Many recently developed mathematical models have aided computations of capture zones, groundwater pathlines, flushing rates, and associated travel times to extraction wells or drains [3], [4], [6], [7], [18], [26], [30], [40], [42], [47], [49], [50], [51]. These models provide insight into patterns generated by alternative pump and treat schemes, and the selection of monitoring locations and frequency.

### **II.3 Optimization and Decision Analysis**

The following articles provide important ideas and theory on determining optimal solutions to groundwater remediation problems given various objectives. Well locations, pumping rates, parameter uncertainty factors, and the baseline methodology are all aspects of each theory that attempts to produce an optimal solution, or in the case of decision analysis, the best available alternative. These solutions are for questions on remediation and containment, which seem to be universal objectives. Not until arriving at Hartman and Schmitt references, are there attempts made to optimize switching periods in pulsed pumping operations.

Huang and Meyer present a new optimization formulation for dynamic groundwater remediation management by simultaneously using well locations and corresponding pumping rates as decision variables [29]. Optimal well locations and pumping rates obtained with the moving-well model were less expensive than solution obtained with a comparable fixed-well model. Well location optimization was more important than pumping rate optimization. In the general problem considered in this work, pumping rates and well locations are unchanged in testing the methodology.

Ahlfeld and Sawyer developed an optimization model to design capture zones for contaminant containment. Sets of candidate well locations were preselected within and around the contamination plume [1]. After testing several well sets, the authors found that pumping costs could be reduced by 37% by using optimal well location set. The well locations were treated as implicit decision variables. The results suggested that incorporating well location

explicitly in groundwater remediation optimization may improve remediation solutions. A basic assumption made in this work was that the pumping rate would be continuous.

Bear and Sun presented an optimization strategy for pump-treat-injection systems using a multi-stage design with chance constraints [5]. The multi-stage decision process is formulated and solved as a two-level hierarchical optimization model. Costs serve as the objective functional while contaminant concentration and total cleanup time are constraints. The number of wells for both pumping and injection is treated as a decision variable. At the basic level, well locations and pump/injection rates are sought to maximize mass removal of contaminants. At the upper level, the number of wells is optimized with respect to minimal cost, taking maximum contaminant level (MCL) as a constraint. This work avoids the issue of dealing with established well locations and pumping rates, and uses economics as a baseline for the analysis.

Wang and Zheng developed a simulation-optimization model to design groundwater remediation systems under a variety of field conditions [56]. The model incorporated a genetic algorithm and global search techniques with MODFLOW and MT3D and allowed for multiple management periods in which optimal pumping/injection rates vary with time to show the changes in the flow and transport condition during the remediation process. This work was an important move towards handling variability, but is limited by requirements for complete plume location knowledge.

Gorelick reviews the existing groundwater studies and subsequent models developed from these studies[25]. He lays out three primary problems that require further investigation. First is a need for improved hydraulic management models, which account for aquifer

parameter uncertainty. Second is an emphasis on groundwater and groundwater quality management models that incorporate nonlinear constraints. Third is a recommendation for policy evaluation and allocation models to account for broad institutional factors and real system features. Wagner and Gorelick present a methodology for addressing the first of the primary problems stated above[55]. Their methodology couples three processes: (1) a finite-element flow and transport simulation model combined with nonlinear least squares multiple regression for simultaneous parameter estimation, (2) linear first- and second-moment analysis to transfer information about the effects of the uncertainty in parameter estimates to the management model, (3) nonlinear chance-constrained stochastic optimization combined with flow and transport simulation for optimal decision making.

Freeze et al. developed a methodology for designing hydrogeological projects and address uncertainty[19]. The methodology is applicable to designs of containment structures for waste management facilities, purge-well networks in contaminant remediation applications, or drainage systems in geotechnical projects. The methodology couples three separate models: a decision model based on a risk-cost-benefit objective function, a simulation model for groundwater flow and transport, and an uncertainty model that encompasses both geological and parameter uncertainty. The strength of this work is in handling uncertainty and unknown conditions. However, it does not determine optimal solutions.

#### **II.4 Pulsed Pumping**

Pulsed pumping method for pump-and-treat technology is a technique that has potential application in remediating contaminated ground water, particularly in the presence of rate-limited sorption and tailing. Keely et al proposed a pulsed pumping method of oper-

ation where the hydraulic well system is cycled through “resting” (pump off) and “active” (pump on) periods[31]. Theoretically, the resting mode would allow sorbed contaminant to diffuse into more mobile regions. When the active mode occurs, contaminant concentrations would be higher.

Harvey et al. concluded that pulsed pumping does not remove more contaminant mass than pumping at a continuous time-averaged rate for a given volume of extracted water[28]. They also found that pulsed pumping removes much less mass than pumping at the continuous time-averaged rate if the resting period is too long. Finally, if pulsed pumping and continuous rates are the same, pulsed pumping will take longer, but will require significantly less time of pump operation. Their conclusions point to a preference for reduced, continuous pumping rates when tailing occurs. Pulsed pumping may be used, however, after installation because continuous pumping at the design rate is impossible or inefficient, and the remediation system will not function effectively at a lower pumping rate. Their calculations produced a dimensionless time interval for pumping as

$$\tau_{pump} = \frac{\pi b \theta d^2 \phi \bar{C}_D(\rho = \rho_0)}{s} \quad (12)$$

and for a maximum resting period of

$$t_{rest} = \frac{2.3}{(k_1 + k_2)} \quad (13)$$

where  $b$  is aquifer thickness,  $\theta$  is the effective porosity,  $d$  is dispersivity,  $\phi$  is dimensionless pumping rate, and  $\bar{C}_D(\rho = \rho_0)$  is the dimensionless concentration at the well [28]. The Laplace parameter is  $s$  and two rate coefficients are  $k_1$  and  $k_2$  for sorption and desorption.

If pulsed pumping is necessary, it can be scheduled to be as efficient as a system designed to pump at a lower rate. Finally the authors concede that pulsed pumping may be

preferred because of savings in operation, labor, or shared costs of treatment system due to the reduced pumping time.

## II.5 Optimized Pulsed Pumping

Hartman began an effort to mathematically analyze pulsed pumping schedules, instead of using the often-used numerical approach [27]. He was able to prove theoretically that an optimal pulsed pumping solution exists for an idealized, radially symmetric aquifer. His hypothetical aquifer used a contaminant transport model affected by rate-limited sorption. He used classical variational calculus to optimize an objective functional and determined necessary and sufficient optimality conditions to obtain the best pulsed pumping schedule for a specific cleanup objective [22]. He ignored contaminant transport due to a natural hydraulic gradient, and he assumed the aquifer thickness to be constant and saturated within the aquifer domain. Contaminant was radially symmetric throughout the vertical extent of the aquifer and a fully penetrating extraction well was placed in the center of the contaminated region. The aquifer was singular and extended to infinity in all directions. No other contaminant sources or sinks existed. Rate-limited sorption was represented with a first order differential equation. Finally, the pumping schedule was piecewise constant on a fixed, finite time interval where only one pulsed pumping cycle was investigated.

In an extension of the efforts by Hartman, Schmitt also used a variational optimization technique to acquire an optimal schedule of pulsed pumping operations, but in a setting for more general applications to existing pump-and-treat aquifer remediation sites [48]. A generic management objective functional is constrained by the contaminant transport equations in two-dimensional (2-D) or three-dimensional (3-D) models, which account

for rate-limited sorption. First variation provides necessary optimality conditions that must be met by any optimal solution, in turn, leading to a pulsed pumping schedule of operation. The second variation provides necessary and sufficient optimality conditions that characterize the solution as minimal, maximal, or neither. The following subsection presents work covered by Schmitt in developing the optimization method using calculus of variations.

### II.5.1 Optimization Problem Statement

The analysis developed by Schmitt and Hartman merged in the case of functionals independent of the temporal variation in concentration. The objective functional,  $J[Q, c]$ , was posed in the form of

$$J[Q, c] = \int_0^{t_f} \int_{B_w} f(t, Q(t), c(\mathbf{y}, t)) d\mathbf{y} dt. \quad (14)$$

This integral represents a generic management objective that can be established for a particular goal of cleanup.

The optimization is a maximization of  $J[Q, c]$  subject to the constraints presented by equations (6), (7), (8), (9), and (11).

However, in order to work the optimization problem, revised theorems must be restated. In Schmitt's dissertation, the necessary optimality conditions for the first variation become

$$[\hat{f} - \hat{c}\hat{f}_c]|_{\mathbf{x}=\mathbf{x}_w}|_{\hat{t}_i=0}^{\hat{t}_i=0} = 0. \quad (15)$$

The sufficient optimality conditions for the second variation become

$$f_{cc}(t, \hat{Q}^{(i)}(t), \hat{c}^{(i)}(\mathbf{x}_w, t)) < 0. \quad (16)$$

Schmitt revised his Theorems 9 and 10 to handle the nonpositive characteristic of the Lagrangian. Now for the optimization problem consider Theorem 1 [48].

**Theorem 1 (Schmitt).** *Suppose that for some admissible functions  $(\hat{Q}, \hat{c}, \hat{\lambda})$  the Lagrangian for the optimization problem established by (6) through (9), (11), and (14) satisfies the following conditions:*

1. The functions  $(\hat{Q}, \hat{c}, \hat{\lambda})$  are an extremal, and hence the first variation of the Lagrangian vanishes.
2. For the functions  $(\hat{Q}, \hat{c}, \hat{\lambda})$ ,

$$R^{(i)}(t) = \frac{1}{2} f_{cc}(t, \hat{Q}^{(i)}(t), \hat{c}^{(i)}(\mathbf{x}_w, t)) < 0 \quad (17)$$

for all  $t \in [t_{i-1}, t_i]$ , and for all  $i = 1, 2, \dots, n$ , and

$$\mathbf{M}^{(i)} \leq 0 \quad (18)$$

for all  $i = 1, 2, \dots, n-1$ , where  $\mathbf{M}^{(i)}$  is given as

$$\mathbf{M}^{(i)} = \frac{1}{2} \begin{bmatrix} \hat{f}_t - \hat{f}_c \hat{c}_t|_{t_i+0}^{t_i-0} & \hat{f}_c|_{t_i+0}^{t_i-0} \\ \hat{f}_c|_{t_i+0}^{t_i-0} & 0 \end{bmatrix}_{\mathbf{x}=\mathbf{x}_w}$$

and

$$m_{11}^{(i)} = \frac{1}{2} [\hat{f}_t - \hat{f}_c \hat{c}_t]_{\mathbf{x}=\mathbf{x}_w}|_{t_i+0}^{t_i-0} \leq 0.$$

where hatted functions imply evaluation at  $\hat{Q}(t)$  and  $\hat{c}(\mathbf{x}_w, t)$ .

3. The time interval  $[t_{i-1}, t_{i+1}]$ , contains no times which are conjugate to the time  $t_{i-1}$ , for all  $i = 1, 2, \dots, n$ .

Then the functional in (14), constrained by the conditions in (6) through (9), and (11) has a maximum at  $(\hat{Q}, \hat{c}, \hat{\lambda})$  with respect to the norm,  $\|*\|_{\tilde{J}}$ .

For this problem, given the functions  $(\hat{Q}, \hat{c}, \hat{\lambda})$  are extremal, the necessary conditions which generate the candidate optimal pulsed pumping schedule become

$$f(t_i, \hat{Q}^{(i)}, \hat{c}(\mathbf{x}_w, t_i)) - f(t_i, \hat{Q}^{(i+1)}, \hat{c}(\mathbf{x}_w, t_i)) - \hat{c}(\mathbf{x}_w, t_i) [f_c(t_i, \hat{Q}^{(i)}, \hat{c}(\mathbf{x}_w, t_i)) - f_c(t_i, \hat{Q}^{(i+1)}, \hat{c}(\mathbf{x}_w, t_i))] = 0 \quad (19)$$

for all  $i = 1, 2, \dots, n - 1$ , where  $\hat{Q}^{(i)}$  and  $\hat{Q}^{(i+1)}$  are stated by equation (20) for the pumping schedule

$$Q^{(i)}(t) = \begin{cases} Q_{on} & \text{for } t \in (t_{i-1}, t_i) \\ 0 & \text{for } t \in (t_i, t_{i+1}) \end{cases} \quad (20)$$

for  $i$  odd integers of the extremal of  $\hat{Q}$ .

### II.5.2 Essential Concentration Function

This optimization problem requires another explanation regarding contaminant concentration. One of the management constraints is to prevent concentrations above a certain level from crossing a regulatory boundary (the proverbial “line in the sand”). Let  $c_s$  represent this as a regulatory level of interest. The essential concentration function,  $\xi(c)$ , is defined as any function of the concentration at the extraction well, such that  $\xi(c)$  is positive for all concentrations above  $c_s$ , and  $\xi(c)$  is negative for all concentrations below  $c_s$ . Further,  $\xi(c_s) = 0$  and the units of  $\xi(c)$  are contaminant mass per volume of the water phase [M/L<sup>3</sup>]. Because of the essential concentration function, the integrand of  $J[Q, c]$  is independent of the time derivative of the concentration, and thus our interest in the form given in equation (14). In other words, the essential concentration function is any function that can represent a remediation manager’s preference for concentrations that are below the regulatory level as a negative number. Concentrations above the regulatory level are rep-

resented as positive numbers. The essential concentration function can take any form, just as long as it passes through zero at the standard concentration or regulatory level. Schmitt started with the form

$$\xi(c) = \eta(\sigma c)^2 + \nu(\sigma c)^3 \quad (21)$$

where  $\eta$  and  $\nu$  are constants which are chosen to satisfy some drinking water standard for the contaminant [M/L<sup>3</sup>] and  $\sigma$  is a concentration scaling factor [L<sup>3</sup>/M] such that  $(\sigma c)$  represents the scaled, dimensionless concentration. This essential concentration function meets the general management preferences with respect to groundwater contamination.

### II.5.3 Necessary Optimality Conditions

The boundary of the well in integral form can be redefined in two dimensions such that this boundary integral becomes the line integral around  $\Gamma_1$

$$\int_{B_w} f dy = \int_{\Gamma_1} f ds \quad (22)$$

where  $s$  is the arclength variable. Now that the theorems are revised to handle the non-positive product of  $\Delta_i^T \cdot \mathbf{M}^{(i)} \Delta_i$ , this problem can now be formalized as a maximization problem:

$$\text{Maximize } J [Q, c] = \int_0^{t_f} \int_{\Gamma_1} f(t, Q(t), c(s, t)) ds dt. \quad (23)$$

constrained by the appropriate conditions given by (6) through (9), and (11), where

$$f(t, Q, c) = -(1 - z)\rho_w [Q + Q_{LO}] + z\xi(c)[Q + Q_{LO}]. \quad (24)$$

The equation (24) is the integrand for the objective function (23). Restated, the integrand is a functional control by the parameters of time, extraction rate (pumping), and concentration. The integrand operates within the objective function so that the objective function is

maximized to determine what the optimal switching times will be in the pulsed pumping operation. The objective function maximum requires necessary optimality conditions and sufficient optimality conditions to confirm that it is a maximum.

In equations (21) and (24),  $\rho_w$  is the density of the water [M/L<sup>3</sup>] and z is a weighting factor [dimensionless] ( $0 < z < 1$ ) introduced because of the large difference between mass of contaminant and mass of water pumped out of the aquifer, and  $Q_{LO}$  is a reduced pumping rate, introduced to maintain hydraulic control of the contaminant plume [L<sup>3</sup>/T].

Combining equations (21) and (24) results in

$$f(t, Q, c) = [(z - 1)\rho_w + z\eta(\sigma c)^2 + z\nu(\sigma c)^3][Q + Q_{LO}]$$

or, alternatively as

$$f(t, Q, c) = [K_0 + K_2(\sigma c)^2 + K_3(\sigma c)^3][Q + Q_{LO}]$$

where  $K_0$ ,  $K_2$ , and  $K_3$  are constants. With this representation for the integrand, we see that  $f$  in equation (24) is analytic in  $c(s, t)$  and thus, if the functions  $(\hat{Q}, \hat{c}, \hat{\lambda})$  are an extremal, they must satisfy the necessary conditions.

The necessary optimality condition from equation (15) restated is

$$[\hat{f} - \hat{c}\hat{f}_c]|_{x=x_w}|_{\hat{t}_i+0}^{\hat{t}_i-0} = 0$$

and becomes

$$\begin{aligned} & \{[K_0 + K_2(\sigma \hat{c})^2 + K_3(\sigma \hat{c})^3][\hat{Q}^{(i)} + Q_{LO}] - \hat{c}[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2][\hat{Q}^{(i)} + Q_{LO}]\}_{\hat{t}_i-0} \\ & - \{[K_0 + K_2(\sigma \hat{c})^2 + K_3(\sigma \hat{c})^3][\hat{Q}^{(i+1)} + Q_{LO}] - \\ & \hat{c}[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2][\hat{Q}^{(i+1)} + Q_{LO}]\}_{\hat{t}_i+0} = 0 \quad (25) \end{aligned}$$

for all  $i = 1, 2, \dots, n - 1$ , and the roots of (25) provide the candidate pulsed pumping schedule. Suppose the extraction pumping is initially on, and we wish to determine the time  $t_i$  to turn the pump off. Then, for this beginning pumping interval we must satisfy

$$\begin{aligned} & \{[K_0 + K_2(\sigma\hat{c})^2 + K_3(\sigma\hat{c})^3][Q_{ON} + Q_{LO}] - \hat{c}[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2][Q_{ON} + Q_{LO}]\}_{t_i=0} \\ & - \{[K_0 + K_2(\sigma\hat{c})^2 + K_3(\sigma\hat{c})^3]Q_{LO} - \hat{c}[2K_2\sigma^2\hat{c} + 3K_3\sigma^3\hat{c}^2]Q_{LO}\}_{t_i+0} = 0. \end{aligned} \quad (26)$$

Since  $\hat{c}$  is continuous at  $t = t_i$ , then  $\hat{c}^{(1)}(\mathbf{x}_w, t_1-0) = \hat{c}^{(2)}(\mathbf{x}_w, t_1+0)$  and the candidate switching time,  $t_1$ , is the first zero of the function  $G(t)$ , defined as

$$G(t) = [K_0 - K_2(\sigma\hat{c})^2 - 2K_3(\sigma\hat{c})^3], \quad (27)$$

where  $\hat{c} = \hat{c}^{(1)}(\mathbf{x}_w, t_1)$ , and the concentration information at the well could be provided by any contaminant transport model which incorporates linear, rate-limited sorption with the extraction well on. Notice, if we wish to determine the next time to turn the pump on, then the zero of the  $G(t)$  again provides the candidate switching time, however now the concentration information is provided by the model with the extraction well turned off.

#### II.5.4 Sufficient Optimality Conditions

According to the second theorem from Schmitt's work, we need  $R^{(i)}(t)$  to be negative on the  $i^{\text{th}}$  interval for every  $i$ . For the partial functional considered here, the inequality condition in equation (17) becomes

$$f_{cc}(t, \hat{Q}^{(i)}(t), \hat{c}^{(i)}(\mathbf{x}_w, t)) = 2\sigma^2[K_2 + 3K_3(\sigma\hat{c})][Q^{(i)}(t) + Q_{LO}] < 0 \quad (28)$$

for all  $t \in [t_{i-1}, t_i]$ , and for  $i = 1, 2, 3$  and 4. If  $Q_{LO}$  is chosen to be a small positive constant, then the constraint in (28) becomes

$$[K_2 + 3K_3(\sigma\hat{c})] < 0 \quad (29)$$

for all  $t \in [t_{i-1}, t_i]$ , and for  $i = 1, 2, 3$  and  $4$ .

## **II.6 Numerical Modeling**

Modeling has become a predictive management tool for site investigations to evaluate remediation strategies, estimate hydrogeological parameters, and understand aquifer and contaminant plume characteristics. For modelers, a site-investigation strategy must be based on answers to three questions: (1) What should be measured? (2) How many measurements should be made? (3) Where should the measurements be located? [20]. Groundwater hydrologists often use models to predict the behavior of groundwater systems. Although some decisions can be made using best engineering or best geological judgement, in many instances human reasoning alone is inadequate to synthesize the conglomeration of factors involved in analyzing complex groundwater problems [2]. The best tool available to help groundwater hydrologists meet the challenge of prediction is usually a groundwater model.

### **II.6.1 Groundwater Modeling System (GMS)**

The Department of Defense's Groundwater Modeling System (GMS) was developed by the Engineering Computer Graphics Laboratory of Brigham Young University. Later versions have been released by support personnel located at the US Army Corps of Engineers, Waterways Experiment Station, Coastal and Hydraulics Laboratory in Vicksburg, Mississippi. GMS was designed as a comprehensive groundwater modeling environment, which creates useful graphical interfaces between popular flow and transport models. Several types of software models are supported and interfaces are established for sharing and transferring information between models and data types. GMS includes tools for site char-

acterization, model conceptualization, mesh and grid generation, geostatistics, and post-processing. The latest version is 2.1 and uses basic platforms MODFLOW and FEMWATER. To model contaminant transport MT3D is used in conjunction with MODFLOW.

### **II.6.2 MODFLOW**

In this thesis, the code used within GMS for basic flow is MODFLOW. McDonald and Harbaugh developed the MODFLOW code in 1984 using Fortran 66 language and later updated it in 1988 using Fortran 77 language [37]. MODFLOW, a numerical model, uses a three-dimensional, finite-differences method. A computer using this model can solve a set of algebraic equations generated by approximating the partial differential equations (governing equations, boundary conditions, and initial conditions) that form the mathematical model [2]. Finite difference methods use a node centered grid system for establishing the aquifer model. Finite difference methods also compute a value for the head at the node, which also is the average head for the cell that surrounds the node. No assumption is made about the form of the variation of the head from one node to the next.

### **II.6.3 MT3D**

Within GMS a transport code is required to simulate concentrations and migration of contaminants, and MT3D provides this capability. The code MT3D is a particle tracking code with advection, dispersion, and chemical reactions of dissolved constituents that are compatible with MODFLOW. The MT3D transport code uses a mixed Eulerian-Lagrangian approach to the solution of the three-dimensional advective-dispersive-reactive equation in three basic options: the method of characteristics (MOC), the modified method of characteristics (MMOC), and a hybrid of these two methods (HMOC) [59]. The dispersion cal-

culations are solved using explicit finite-difference methods. The approach taken in this thesis combines the strength of the method of characteristics for eliminating numerical dispersion and the computational efficiency of the modified method of characteristics. This selective use of HMOC has made simulation relatively accurate and meaningful. Retardation is incorporated into the particle-tracking and dispersion calculations explicitly. Heads and cell-to-cell flux terms are computed by MODFLOW during this simulation phase and are written to a specially formatted document (for hydraulic heads). MT3D retrieves it and automatically incorporates the specified hydrologic boundary conditions. The code accommodates a variety of spatial discretization capabilities and transport boundary conditions including: (1) confined, unconfined variably confined/unconfined aquifer layers, (2) inclined model layers and variable cell thickness within the same layer, (3) mass flux boundaries, and (4) the solute transport effects of external sources and sinks such as wells, drains, rivers, areal recharge, and evapotranspiration.

## **II.7 Contaminant Properties**

To attempt an accurate representation of contaminant transport behavior, details of the aquifer alone are insufficient to completely develop the necessary inputs. Contaminants can be generally divided into groups including synthetic organic chemicals, hydrocarbons, inorganic cations, inorganic anions, pathogens, and radionuclides [17]. One subset of the hydrocarbons is the halogenated hydrocarbon. Most halogenated hydrocarbons dissolve to some degree and typically create dual aqueous and non-aqueous phase liquids. Dissolution lends the contaminant to transport within the aquifer. This work has selected carbon

tetrachloride as the contaminant of interest, and hydrogeological parameters will show this consideration.

Carbon tetrachloride is a halogenated hydrocarbon and has been used as a degreaser, refrigerant/propellant, fumigant, and in chemical manufacturing [13], [17]. Table 2 lists characteristics of carbon tetrachloride [13].

Groundwater contamination is a long-term problem. Acceptable in the past, management practices allowed some wastes to be buried, dumped, leaked, etc. and it has taken decades to rediscover. Although many groundwater-contamination sites are small, some sites are fairly extensive due to the long time period over which contamination has been migrating away from the source [17].

Compound	Boiling Pt.	Solubility	Log K <sub>ow</sub>	Fish Toxicity LC <sub>50</sub>	WHO	MCL
Carbon tetrachloride	77 deg C	785 mg/L	2.70	50 mg/L (20 hr)	2 $\mu$ g/L	5 $\mu$ g/L

Table . 2. Physical Properties and Limits

### III. Methodology

#### III.1 Overview

The work presented in this document applies and further extends the mathematical tool developed by Hartman and Schmitt. Some changes are necessary for the objective function, and additionally, physical constraints are added to make the methodology more robust. The remainder of this chapter develops the simulation model and presents the modeling process in detail. Important simulation considerations are addressed including advection/dispersion, sorption, diffusion, and numerical setting in the numerical model analysis.

Table 3 describes three problems and how this work relates to previous work. The remainder of this chapter will develop the objective function and necessary constraints required to complete the analysis.

The methodology developed here will fundamentally address the general remediation problem. That is to maximize the essential mass removed while minimizing the non-essential mass removed and the total mass of the water removed. The essential concentration function is derived from the essential and non-essential masses as determined by some prescribed drinking water standard,  $c_s > 0$ .

	Dewater	Containment	Remediation
Schmitt	Not Considered	Not Considered	Issue
This work	Issue	Issue	Issue

Table . 3. Research Coverage

## III.2 Essential Concentration Function

The essential concentration function must meet certain requirements to satisfy general management objectives. In general, the function should equate to zero when the contaminant concentration is at an acceptable level as determined by some regulatory agency. By convention and logic, a negative value should occur when the concentration is below the standard, and a positive value should occur when the concentration is above the standard. This leads to the question of mathematically representing the function, and its exact form. First, we will add a definition to the theory to help establish the basic requirements for the essential concentration function.

**Definition:** *We say that  $\xi(\sigma c)$  is an essential concentration function if:*

1.  $\xi(\sigma c)$  is continuous for  $[0, \infty)$ .
2.  $\xi(\sigma c_s) = 0$
3.  $\xi(\sigma c) > 0$  for all  $c > c_s$
4.  $\xi(\sigma c) \leq 0$  for all  $c < c_s$
5.  $\xi(\sigma c)$  is nondecreasing on  $[c_s, \infty)$ .

Point 1 of the definition implies that the essential concentration function behaves normally and rationally with regard to changes in concentrations. Point 2 implies that there is a function or functions such that when the concentration is equal to the standard, the function is zero. Points 3 and 4 imply that the essential concentration function crosses the zero line at the standard concentration to indicate a boundary between acceptable and unac-

ceptable concentrations. Point 5 implies that the higher the concentration gets the greater its impact is on the operation. The essential concentration functions to be used with this methodology must comply with these basic principles to satisfy expectations and requirements from the managerial perspective.

The essential concentration function from equation (21) is restated in a more general, factored form of [48]

$$\xi(c) = (\sigma c)^p (\eta + \nu \sigma c)^q \quad (30)$$

where  $p = 2$ , and  $q = 1$ . The variables  $\eta$  and  $\nu$  were constants chosen to satisfy the drinking water standard for the contaminant. Many questions stand out as requiring an answer about the meaning and form of the essential concentration function. Knowing that it is a management concept, we might obtain a better understanding of the concept by looking at its purpose within the objective function,  $G(t)$ . As noted in Chapter 2, the essential concentration function is an important element of the objective function integrand.

The general form of the integrand is

$$f(t, Q, c) = \{-(1-z)\rho_w + z\xi(c)\}(Q + Q_{LO}).$$

Necessary optimality conditions are found when

$$[\hat{f} - \hat{c}\hat{f}_c]|_{\mathbf{x}=\mathbf{x}_w}|_{t_1=0}^{t_1=0} = 0.$$

Substituting the general form into the optimization

$$\begin{aligned} & \{((z-1)\rho_w + z\xi(c))(\hat{Q}^{(i)} + Q_{LO}) - \hat{c}z\xi'(c)(\hat{Q}^{(i)} + Q_{LO})\}_{t_1=0} - \\ & \{((z-1)\rho_w + z\xi(c))(\hat{Q}^{(i+1)} + Q_{LO}) - \hat{c}z\xi'(c)(\hat{Q}^{(i+1)} + Q_{LO})\}_{t_1=0} = 0 \end{aligned}$$

where  $\xi'(c)$  is the partial derivative with respect to concentration. Given that the pumping is initially active and transitions to resting this equation reduces to

$$\{((z-1)\rho_w + z\xi(c))(Q_{ON}) - \hat{c}z\xi'(c)(Q_{ON})\}_{t_1=0} = 0.$$

Roots occur when

$$(z-1)\rho_w + z\xi(c) - \hat{c}z\xi'(c) = 0. \quad (31)$$

Now, an equivalent form of equation (30), but without the use of  $\eta$  and  $\nu$  can be written as

$$\xi(\sigma c) = g(\sigma c)(\sigma c - \sigma c_s)^q. \quad (32)$$

The use of  $g(\sigma c)$  allows for a larger range of possibilities that may occur. We maintain the root(s) at the point where the concentration and the standard are equal because of the importance of the standard concentration. In most cases the parameter  $q$  must be constrained to be an odd positive integer in order to comply with the definition of the essential concentration function. Later in Chapter 4, we will look a special case were  $q = 2$  and the definition holds.

The partial derivative with respect to concentration is

$$\xi'(\sigma c) = g'(\sigma c)(\sigma c - \sigma c_s)^q + g(\sigma c)q\sigma(\sigma c - \sigma c_s)^{q-1}.$$

Substituting into (31)

$$\frac{(z-1)}{z}\rho_w + g(\sigma c)(\sigma c - \sigma c_s)^q - cg'(\sigma c)(\sigma c - \sigma c_s)^q - g(\sigma c)q\sigma(\sigma c - \sigma c_s)^{q-1} = 0.$$

The function  $G(t)$ , which is the result of the objective function integration, provides candidate switching times and is show here as

$$G(t) = \frac{(z-1)}{z}\rho_w + g(\sigma c)(\sigma c - \sigma c_s)^{q-1}\{(1-q)\sigma c - \sigma c_s\} - cg'(\sigma c)(\sigma c - \sigma c_s)^q. \quad (33)$$

It is interesting to note that since the essential concentration function requires that  $q$  always be an odd integer, the response of the objective function will never cross zero at the concentration equal to the standard. Chapter 4 will examine three forms of the essential concentration function. The first example will analyze the situation where  $g(\sigma c) = (\sigma c)^2$  and  $q = 1$ . The second example will analyze a fifth-order polynomial where  $g(\sigma c) = 1$  and  $q = 5$ . The last example will analyze a parabolic where  $g(\sigma c) = 1$  and  $q = 2$ .

### III.3 Comprehensive Objective Function

#### III.3.1 Development

At issue in this chapter as noted in Table 3, is contaminant containment. A constraint is needed to relate the containment issue to the overall problem. This new  $I(t)$  functional will govern the decisions made using  $G(t)$ . The  $I(t)$  functional relies on concentration measurements taken at a point downgradient from the extraction well such as from a monitoring well and has the form

$$I(t) = c(x_i, t) - c_s. \quad (34)$$

When the concentration at the monitoring well shows compliance, this functional will always be negative. It therefore does not constrain the optimization at the extraction well. Once the functional  $I(t)$  is positive, it takes precedence and pre-empts the pulsed pumping operation with continuous pumping. It is important to note a limitation with the monitoring well that the position  $x_i$  must be within the capture region of the extraction well. At steady-state, the stagnation point marks the limit downgradient of the capture zone. It has

the form

$$\mathbf{x}_{stag} = \frac{-Q_{ON}}{2\pi B} \mathbf{K}^{-1} \frac{\mathbf{m}}{|\mathbf{m}|^2} \quad (35)$$

where  $Q_{ON}$  is the pumping rate,  $\mathbf{K}$  is the hydraulic conductivity,  $B$  is the confined aquifer thickness, and  $\mathbf{m}$  is the regional hydraulic gradient vector without the effect of any pumping wells.

The final concern of this work includes the limitation on the extraction rate. Obviously, if the extraction rate is high enough a well will go dry, at least in the short term. Even prior to this, the drawdown in the well must be limited in order to insure applicability of this pulsed pumping methodology. In a confined well, flow remains horizontal on our general assumptions. If drawdown is great enough to create an unconfined condition within the well, then flow is no longer horizontal and the necessary assumptions become invalid. In this objective  $H(t)$  is given using the Theis equation and has the form

$$H(t) = (h_0 - h) - \frac{Q}{4\pi T} W(u(t))$$

and

$$u(t) = \frac{r^2 S}{4Tt} \quad (36)$$

where  $h_0$  is the initial hydraulic head,  $h$  is the resultant hydraulic head,  $Q$  is the pumping rate,  $T$  is the transmissivity, and  $W(u)$  is the well function. The argument  $u$  is a function of  $r$ , the radial distance from the pumping well,  $S$ , the storativity, and  $t$ , the time since pumping began. The well function is an infinite series, which replaced an integral  $\int_u^\infty \frac{e^{-u}}{u} du$  found in the original Theis equation [16]. Fetter also includes tabulated values of the well function for various  $u$  in his appendix [16].

### III.3.2 The Comprehensive Function

To combine the constraints with our objective, the comprehensive function in general terms will be

$$\hat{Q} = U\{G^*(t), H(t), I(t)\}. \quad (37)$$

The function,  $G^*(t)$  is the combination of both necessary optimality conditions and sufficient optimality conditions from analyzing the roots of  $G(t)$  mentioned earlier. Accordingly, we need ?? to be negative on the  $i^{\text{th}}$  interval for every  $i$ . For the general functional, the inequality condition becomes

$$f_{cc}\{t, \hat{Q}(t), c(x_{w,t})\} < 0. \quad (38)$$

The operation is determined from analysis of the responses. The response to each function will be in simple sign format such that if the function is positive the response is 1, and if the function is negative the response is 0. In tabulated form, the responses are shown in Table 4.

Using logic (Boolean Algebra) the overall response is given by

$$\hat{Q} = H(G^* + I) \quad (39)$$

or using logic operators

$$\hat{Q} = H \wedge (G^* \vee I). \quad (40)$$

### III.4 Aquifer Design

In Schmitt's dissertation, the strategy was tested using a modified version of SUTRA code, which successfully incorporates first and second order diffusion models which emulate rate-limited sorption into a two-dimensional finite element flow and transport model

Response (G*)	Response (H)	Response (I)	Pumping (Q)
1	1	1	1
1	1	0	1
1	0	1	0
1	0	0	0
0	1	1	1
0	1	0	0
0	0	1	0
0	0	0	0

Table . 4. Objective Effects

[11]. The simulation plan for this work will analyze a more complex two-dimensional, aquifer model using MODFLOW and MT3D. Because MODFLOW and MT3D do not incorporate rate-limited sorption, the model design will utilize a clay layer to create an immobile region for exhibiting tailing and rebound characteristics typical of rate-limited sorption. A new package, MT3DMS, which was released in May 1998, does have the ability to emulate rate-limited sorption, but the graphical interface within GMS will not be complete until early summer of 1999.

### **III.4.1 Design in GMS**

Caspers and Schmitt used the same aquifer design within the SUTRA code that Caspers modified [11]. Their hypothetical model was two-dimensional, contaminated, sandy aquifer. The simulation aquifer was modeled after a well known large-scale field experiment conducted at Borden, Canada in August 1982 [21], [34], and [45]. In this work, these conditions will be repeated to some extent, but a few changes are necessary. The GMS aquifer model used here is three-dimensional, but all calculations will essentially be two-dimensional. Because the transport package, MT3D, assumes instantaneous sorption/desorption of contaminant (LEA), the model will include a clay layer to provide a relatively immobile region. MT3D allows adjustment of the ratio of the diffusion rate over the advection rate to a very small number [23]. In addition, an immobile region and a mobile region are used to reproduce tailing and rebound characteristics that normally occur when sorption is rate-limited. To note some of the other changes, the aquifer is assumed confined and has a regional hydraulic gradient of 0.01. A small clay layer is added to this model to compensate for missing rate-limited sorption capabilities, which introduces

some heterogeneity. Initial contaminant was simulated by injection of carbon tetrachloride into the aquifer at a rate of 94.5 m<sup>3</sup>/day, with a concentration of 5.0  $\mu\text{g/l}$ , for a period of 100 days. Following this initial injection, the system was undisturbed for an additional 100 days and transient solute transport was simulated. The short cleanup period followed for 100 days, with the extraction well operating at 200 m<sup>3</sup>/day (arbitrary setting). The last preparatory period of no pumping will allow the contaminant concentration to rebound slightly so that the initial conditions are established just prior to beginning the pumping optimization methodology.

To review, the simulations are divided into two parts. The first part initializes the aquifer and plume characteristics to develop the base hydraulic head and concentration data sets for the entire aquifer. The second part uses established conditions from the beginning stage and provides the experimental platform for testing and obtaining results from the optimization methodology.

#### ***III.4.1.1 Part 1: The Initialization Stage***

Within GMS, the aquifer is developed using a grid approach, and refining the grid spacing to minimum dimensions at the extraction well. The dimensions of the aquifer are 180 meters wide by 270 meters long with the hydraulic gradient following the full length of the aquifer. Time units used within the model are days. Initial conditions set all grid cells within the aquifer as active, with some exceptions. The highest and lowest hydraulic head columns are specified head boundaries. These specified heads are set at 220 meters and 217.6 meters respectively to produce an initial regional gradient of 0.01. The starting head array for the interior of the aquifer is 218.8 meters, which is an average of

the two boundaries to allow for easy convergence. With an array of steady-state head values computed, these values are imported into the initial conditions for the transient simulation run. The overall layout of the hypothetical aquifer and grid system is shown in Figure 1.

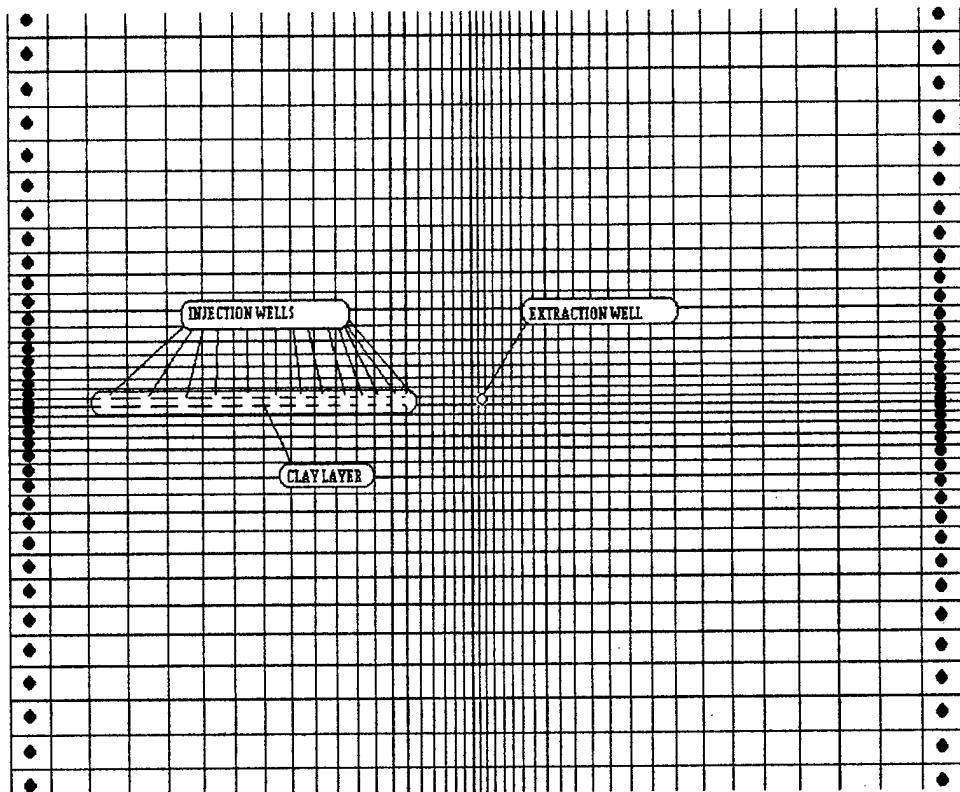


Figure 1. Model Grid Layout (grid centered at extraction well).

The next step is to set the block-centered flow package (BCF). The aquifer concept characterizes the model as confined and having uniform thickness of 20 meters. Because the aquifer is confined, the parameter for hydraulic conductivity is converted to transmissivity. The values used 124.4  $\text{m}^2/\text{day}$  and 0.124  $\text{m}^2/\text{day}$  for the clay layer. The hydraulic head gradient created during the first active period for the extraction well is shown in Figure 2.

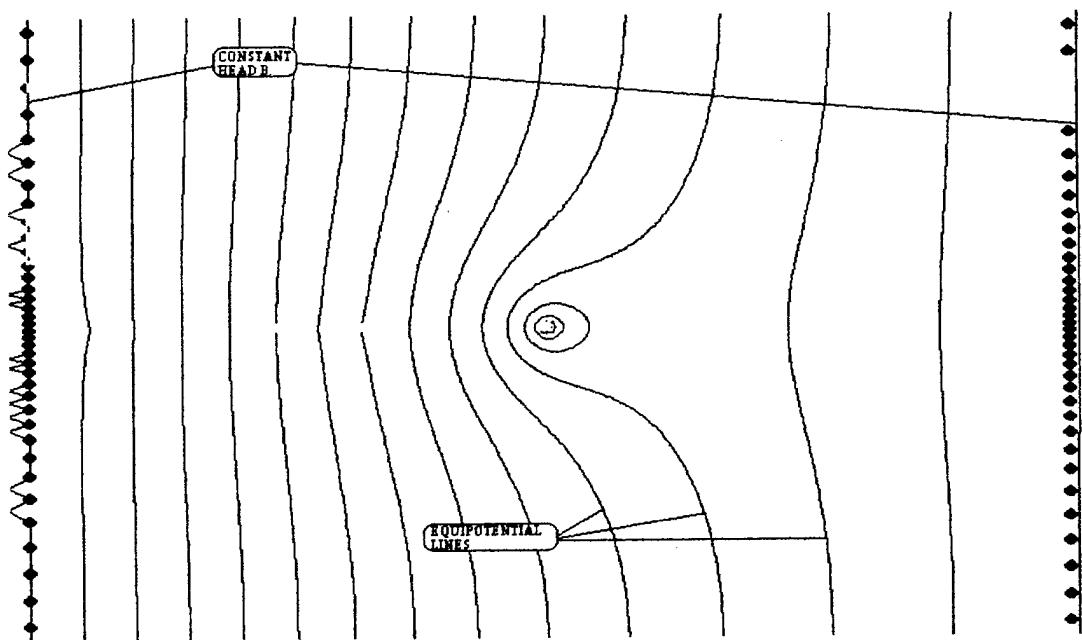


Figure . 2. Hydraulic Gradient (after 300 days).

With the hydraulic setting established, the transport setting can be introduced. The basic transport package also uses the units of days and activates the packages for advection, dispersion, source/sink mixing, and chemical reaction. All cells are activated and initial concentration are zero. The top elevation of the aquifer is set at twenty meters, and again the aquifer thickness is uniform at 20 meters. The porosity array for the aquifer is uniform at 0.33, except for the clay layer where the porosity is set to 0.4. The storativity (1/L) is uniform within the aquifer and is set at  $5 * 10^{-5}$  per meter as a typical value. The clay layer uses  $1 * 10^{-3}$  per meter as typical value.

For the injection wells, the concentration of the contaminant is set to 5 ppb. Fourteen wells were added including thirteen injection wells and one extraction well. One injection well introduces contaminant into the main part of the aquifer at 8.64 cubic meters per day. The other twelve wells inject contaminant into the clay layer in a rates ranging from 5 to 8.64 cubic meters per day for a total of 85.9 cubic meters per day. The extraction well initially withdraws water at 200 cubic meters per day. Table 5 gives a rate schedule for the thirteen injection wells.

The particle tracking algorithm uses the fourth order, Runge-Kutta method. Within the dispersion package, the longitudinal dispersivity is constant for the entire grid at 0.6. The ratio of the transverse dispersivity to the longitudinal dispersivity is set at 0.167. The dispersivity was calibrated from a modeling study of carbon tetrachloride at the aquifer in

Period (days)	Well 1	Well 2	Well 3	Well 4	Well 5	Well 6	Well 7	Well 8
0-100	8.64	8.64	8.64	8.64	8.64	8.64	8.64	7.3
>100	0	0	0	0	0	0	0	0

Table . 5a Injection Well Schedule

Period (days)	Well 9	Well 10	Well 11	Well 12	Well 13
0-100	6.6	6.0	5.5	5.0	8.64
>100	0	0	0	0	0

Table . 5b Injection Well Schedule

Borden, Canada site [34], [21], and [45]. The chemical reaction package requires the last inputs. The sorption option with linear isotherm is enabled. The linear isotherm was chosen because the contaminant concentration is much less than the saturation level by about four orders of magnitude. Bulk density is set to 104.0, the first sorption constant is set at 0.003 and the second sorption constant is set to 0. The mean porosity was set to 0.33. These parameter values are also consistent with the modeling study (appendix A) determinations for retardation and sorption. The solution for the retardation factor,  $r_f$ , is given by

$$1 + \frac{\rho_B}{\theta} K_d = r_f \quad (41)$$

where  $\rho_B$  is the bulk density ( $M/L^3$ ),  $\theta$  is the porosity ( $1/L^2$ ), and  $K_d$  is the distribution coefficient ( $L/M$ ) [17]. The retardation in this model is 1.95. Figure 3 represents a starting point for this work where pulsed pumping and continuous pumping will be compared. The plume boundary is at  $0.02 \mu g/L$ . Concentrations below this value are not visible in the graphical output. The interior contours above the concentration  $2.0 \mu g/L$  are not shown either.

### ***III.4.1.2 Part 2: The Methodology Testing Stage***

The transport solution from above provides the setting for engaging the simulation with the optimal pulsed pumping strategy. The solution that generated concentrations throughout the aquifer are imported as a starting point for the second part of the simulation. At this point, the simulation is divided into stress periods which alternate the pumping operations between active and resting periods. Concentrations are measured and transferred to the optimization function to determine optimal switching times for the pump. In

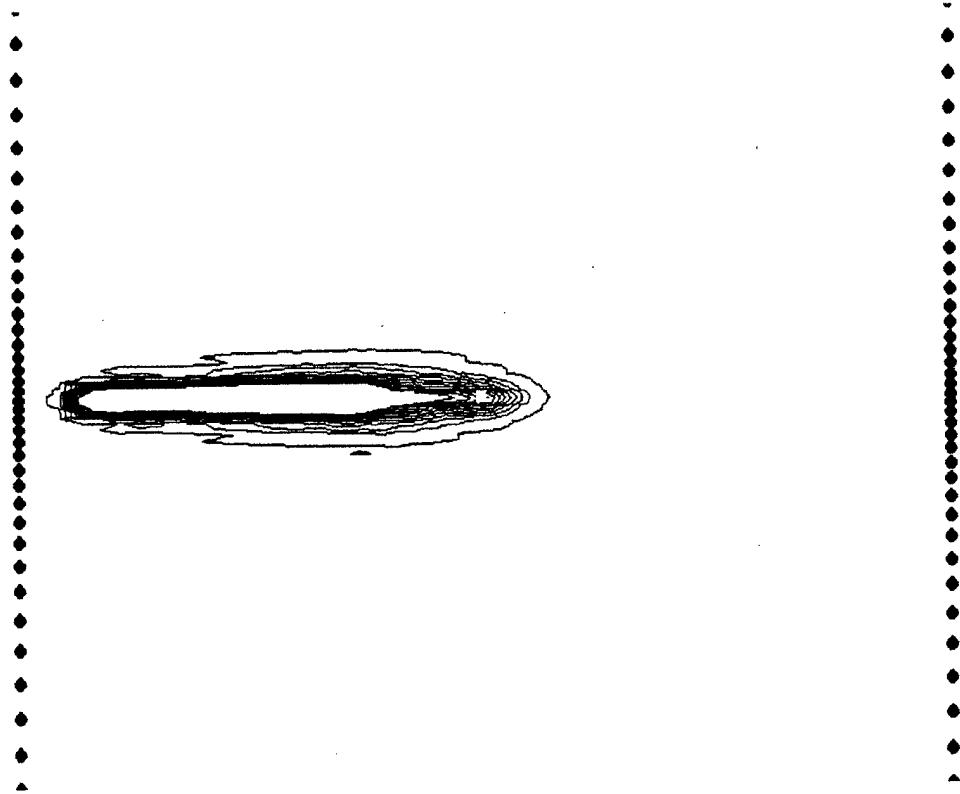


Figure . 3. Plume at 420 days (displayed down to 20 micrograms per cubic meter).

addition, a second simulation which uses continuous pumping rate will be carried out for comparison.

Considering that 420 days has passed within the simulation, greater knowledge about the plume and the hydrological parameters is assumed. Given this increased knowledge, a better pumping rate can be determined using the model aquifer parameters and the existing plume footprint. At a point about 10 meters up-gradient from the extraction well the plume is approximately 20 meters wide. Field experiences generally deal with a large amount of uncertainty regarding the plume dimensions, and seasonal influences will also contribute to variation in plume migration [45]. Given the typical uncertainty, the capture zone will be required to be about twice the plume width. Using capture zone equations an appropriate pumping rate of  $76 \text{ m}^3/\text{day}$  is selected for the purposes of this study [30] and [16]. Appendix A applies the capture zone theory to reduce the  $200 \text{ m}^3/\text{day}$  pumping rate to a lower rate of  $76 \text{ m}^3/\text{day}$ .

The essential concentration used in this study will be  $2000 \mu\text{g}/\text{m}^3$ , which is the guideline limit recommended by WHO for carbon tetrachloride found in drinking water.

## IV. Applications

### IV.1 Essential Concentration Function and Objective Function

#### IV.1.1 Example 1

Example 1 is the first of three possible essential concentration functions that could be chosen as the integrand for the objective function. Each form has unique behavior with respect to a range of concentrations. The concept relates back to the remediation program manager's value considerations. For instance, managers could have varying degrees of aversion to concentrations above the regulatory level. The form could also be swayed by the type of contaminants present and the level of risk to the surrounding environment. In all there are many possible influences on the essential concentration function and subsequent influence on the objective function. The effort here is illustrate the consequences of selecting different forms for the essential concentration function.

Substitution into equation (33) with  $g(\sigma c) = (\sigma c)^2$  and  $q = 1$  will be the first problem analyzed. In this case we will re-analyze the use of the third-order polynomial form, but in more general terms. The general for the essential concentration is

$$\xi(\sigma c) = (\sigma c)^2(\sigma c - \sigma c_s). \quad (42)$$

Combining this essential concentration function with the general equation (33), the result is

$$G(\sigma c) = \frac{(z-1)}{z} \rho_w + \sigma c_s (\sigma c)^2 - 2(\sigma c)^3. \quad (43)$$

Figure 4 shows  $G(c)$  response over a range of scaled concentrations. Two real, positive roots occur at the scaled values of 9.2 and 17.9. See Appendix B for spreadsheet layout

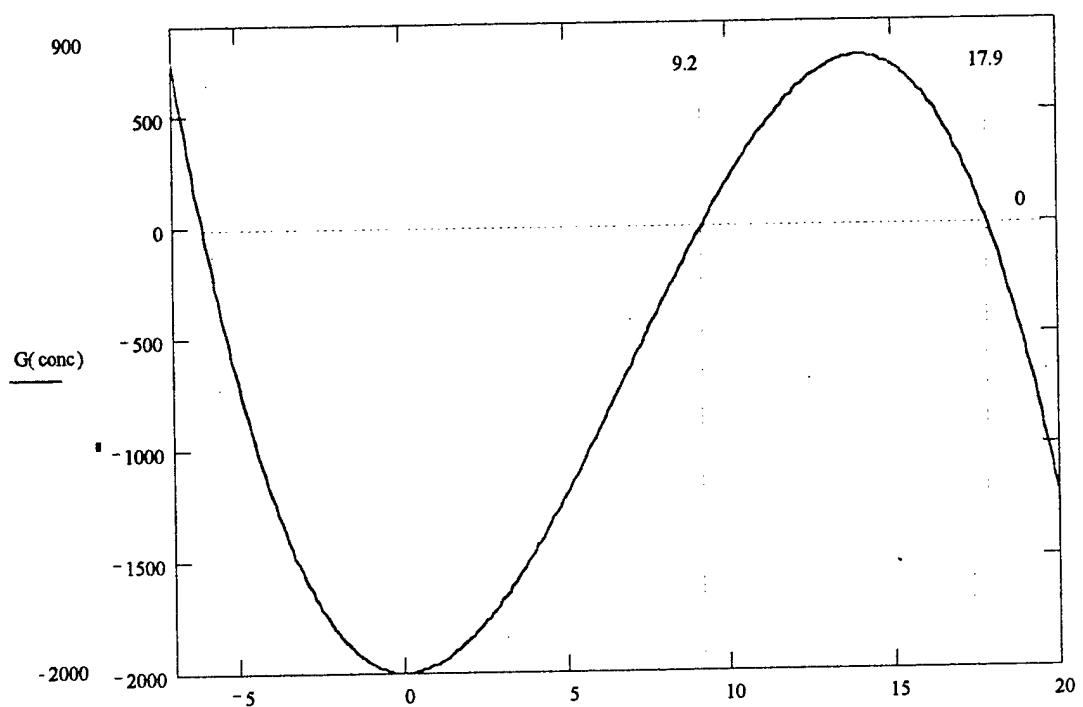


Figure . 4. Third-order polynomial function response.

and calculations for Example 1. This form of the essential concentration function fits the definitions from Chapter 3 and provides the necessary roots needed for the objective function.

#### IV.1.2 Example 2

The essential concentration function can take other forms of higher order polynomials. In this case one possible alternative, the fifth-order polynomial, is selected as a possible essential concentration function. Selection of this type of function offers a significant response in cases of very high concentration or very low concentration relative to the standard concentration,  $c_s$ , and relative insensitivity at concentrations close to the standard. The equation (44) is shown as

$$\xi(c) = (\sigma c - \sigma c_s)^5. \quad (44)$$

Using the function (44), the  $G(c)$  function becomes

$$G(c) = \frac{(z-1)}{z} \rho_w + (\sigma c - \sigma c_s)^4 [(-4)(\sigma c) - \sigma c_s]. \quad (45)$$

Working through the expansion of equation (45) provides

$$G(c) = K_0 - 10K_2(\sigma c)^2 - 20K_3(\sigma c)^3 - 15K_4(\sigma c)^4 - 4K_5(\sigma c)^5.$$

The  $K_i$  constants are used to simplify the expression and are defined in Table 6 as:

Figure 5 shows  $G(c)$  response over a range of scaled concentrations (dimensionless).

$K_0 =$	$(z-1)\rho_w - \sigma^5 c_s^5 z$
$K_1 =$	0
$K_2 =$	$-\sigma^3 c_s^3 z$
$K_3 =$	$\sigma^2 c_s^2 z$
$K_4 =$	$\sigma c_s z$
$K_5 =$	$z$

Table . 6. Coefficient Table.

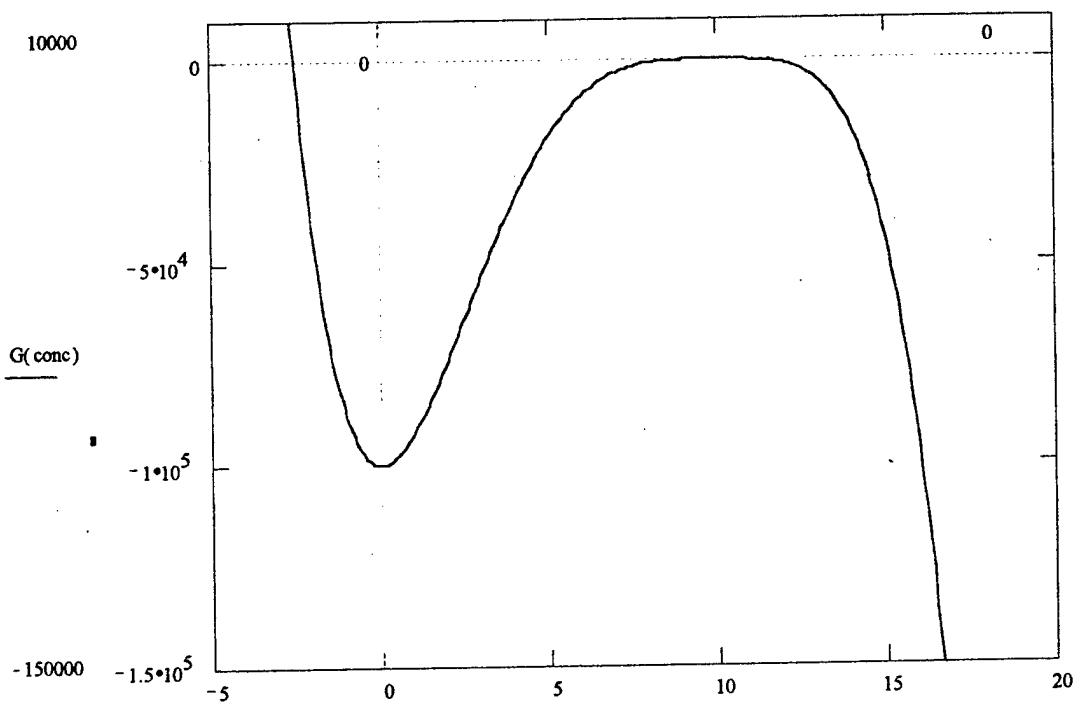


Figure . 5. Fifth-order polynomial function response.

This form meets all of the definition requirements, but unfortunately has only one real root, and its negative. Given this type of essential concentration function the non-interesting solutions requires continuous pumping. Varying the scaling factors does not produce real positive roots with this form. The one real root in this example corresponds to negative concentrations that are physically impossible. See Appendix C for spreadsheet layout and calculations for Example 2.

#### IV.1.3 Example 3

Another consideration for an essential concentration function is the parabolic form.

$$\xi(\sigma c) = (\sigma c - \sigma c_s)^2. \quad (46)$$

The  $G(c)$  function has the form

$$G(c) = \frac{(z-1)}{z} \rho_w + \sigma^2 c_s^2 - 2\sigma c_s (\sigma c) + (\sigma c)^2. \quad (47)$$

Figure 6 shows  $G(c)$  response over a range of scaled concentrations (dimensionless). This response also produces a non-interesting solution to the objective function. The sufficient optimality conditions for the initial switching time coincide with negative concentrations. No amount of pumping would ever produce a negative concentration, and as a result, the solution is continuous pumping. See Appendix D for spreadsheet layout and calculations for Example 3.

### IV.2 Modeling Results

#### IV.2.1 Concentration Data

Using the essential concentration function and objective function from Example 1, which involves the third-order polynomial function, the methodology is used to determine

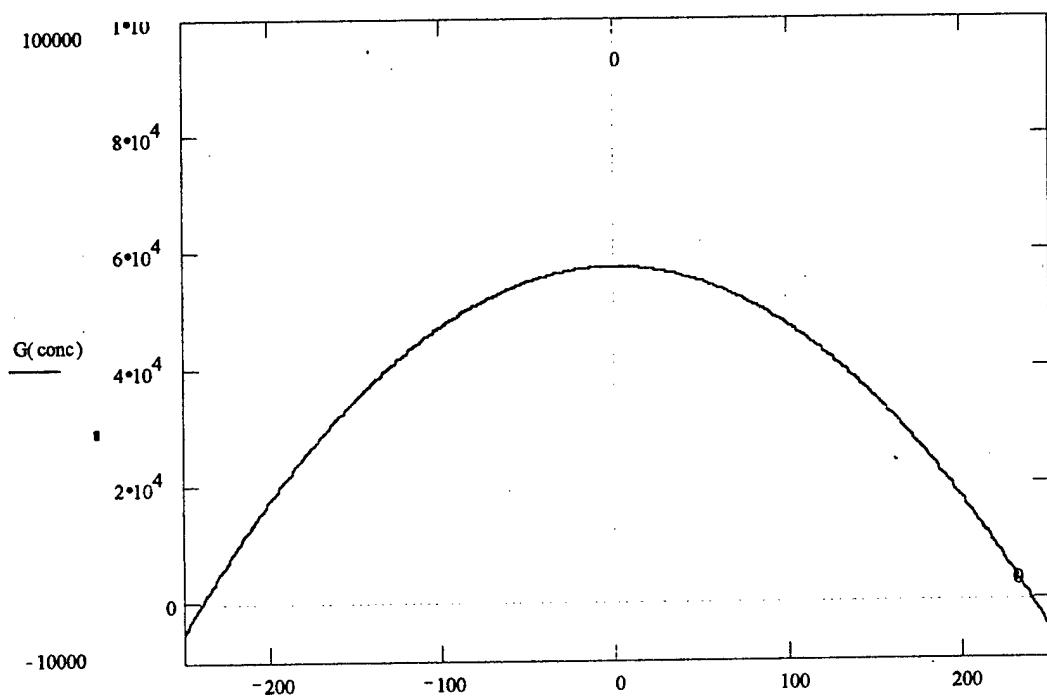


Figure . 6. Parabolic function.

an optimal pumping schedule. Table 7 shows the results that indicate an optimal solution involves switching times and thus pulsed pumping. The methodology determined optimal switching times from measuring concentrations at the extraction well and identifying the emergence of necessary and sufficient optimality conditions. The time units used in the simulation were days. The time unit of days caused overshoot of the exact optimal switching time. In order to be more precise in the switching time, the time units would have to become hours. To change time units from days to hours, the computational load would have increased severalfold. For the purposes of this investigation, the accuracy available in the time units of days was considered acceptable.

Figure 7 details the response from the objective function. Ideally, the response should appear like of series of "humps" with minimums resting on the zero line. The simulation provided more realism by not producing ideal conditions, and to be explained later, supports the robustness of the methodology. Figure 8 represents a time series plot of concentration at the extraction well. The cumulative mass budget results for the simulation are recorded in Table 8. In Table 8 all measurements are masses measured in milligrams. Excerpts of output files from MODFLOW and MT3D are located in Appendix E.

The discrepancy above should be noted as a difference of 0.96%. Next the simulation was run again, but with continuous pumping schedule. The concentration behavior at the extraction well is seen in Figure 9.

The mass balance calculation for this simulation indicated a discrepancy of 1.1%. In comparison between pulsed pumping and continuous pumping, the continuous pumping removed 13.9% of the mass and the pulsed pumping removed 13.2% of the mass. The

Switching Time	Project Day	Concentration ( $\mu\text{g}/\text{m}^3$ )
$t_0$	0	1,686
$t_1$	50	424
$t_2$	70	851
$t_3$	102	427
$t_4$	123	906
$t_5$	141	410
$t_6$	155	853

Table . 7. Switching Times and Observed Concentrations

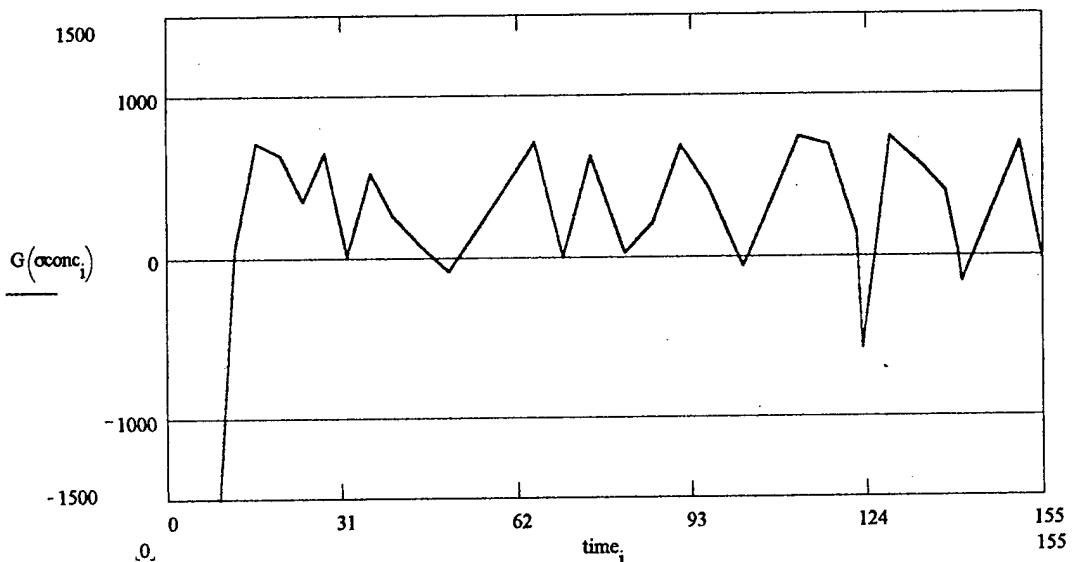


Figure . 7.  $G(t)$  time series for pulsed pumping.

	In	Out
Constant Head	0	1.06E-7
Wells	49.779	-14.787
Decay/biodegradation	0	0
Storage (solution)	32.029	51.848
Storage (adsorbed)	29.385	45.628
Total	111.19	112.26

Table . 8. Mass Budget

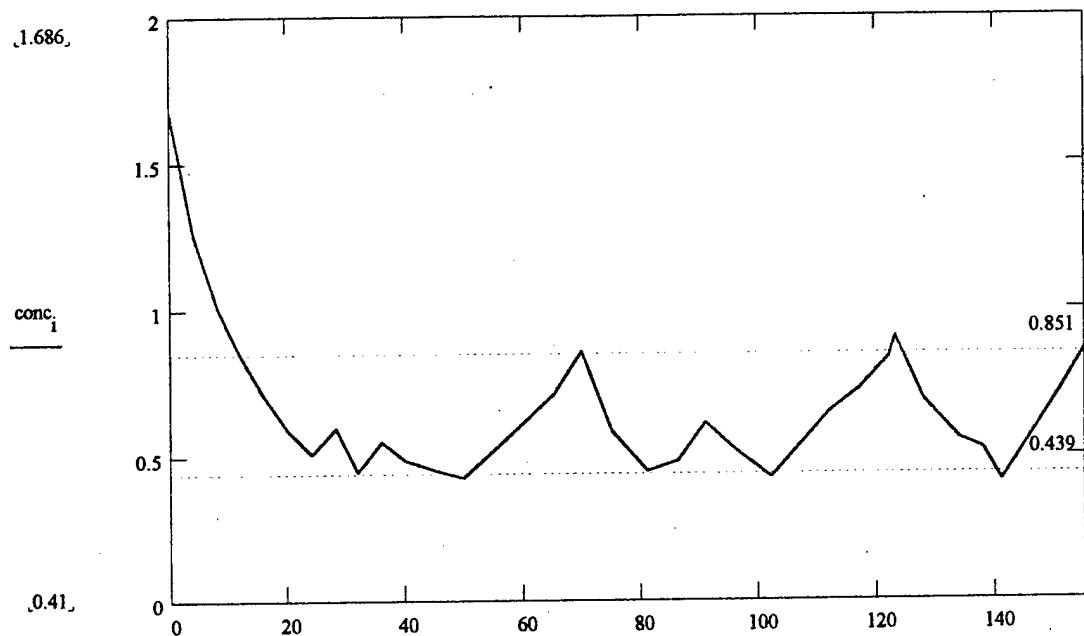


Figure . 8. Extraction well concentration under pulsed pumping.

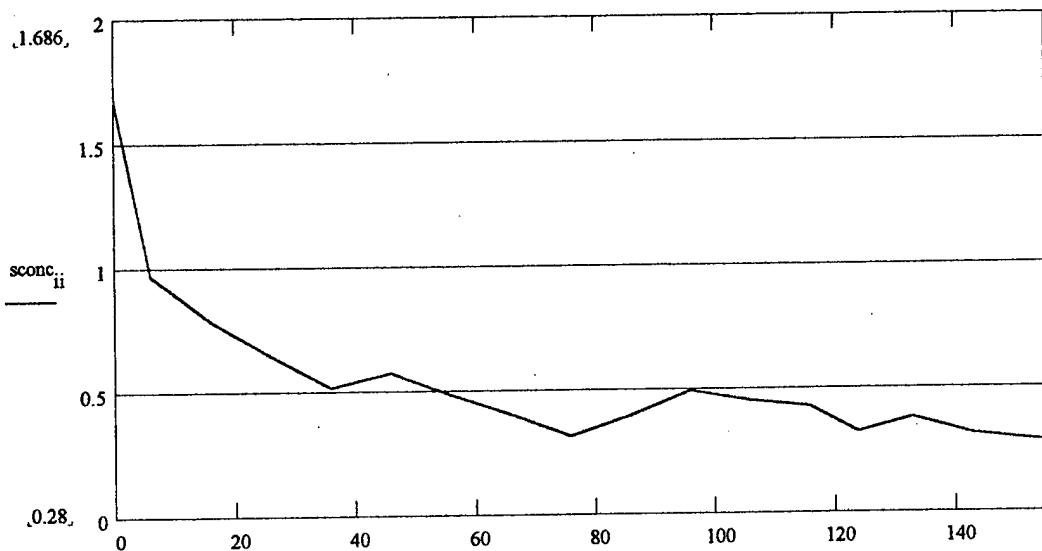


Figure . 9. Extraction well concentration for continuous pumping at 76 m<sup>3</sup>/day.

increase in mass removed per cubic meter of water by going to the pulsed pumping method is 47.2%, and the pump was at rest for 55 of the 155 days.

Harvey et. al. stated that a time-averaged pumping rate would be at least as effective as pulsed pumping [28]. Considering their proposal, the time-averaged pumping rate was determined to be 49 cubic meters per day over 155 days. Figure 10 presents concentrations at the extraction well during this time period.

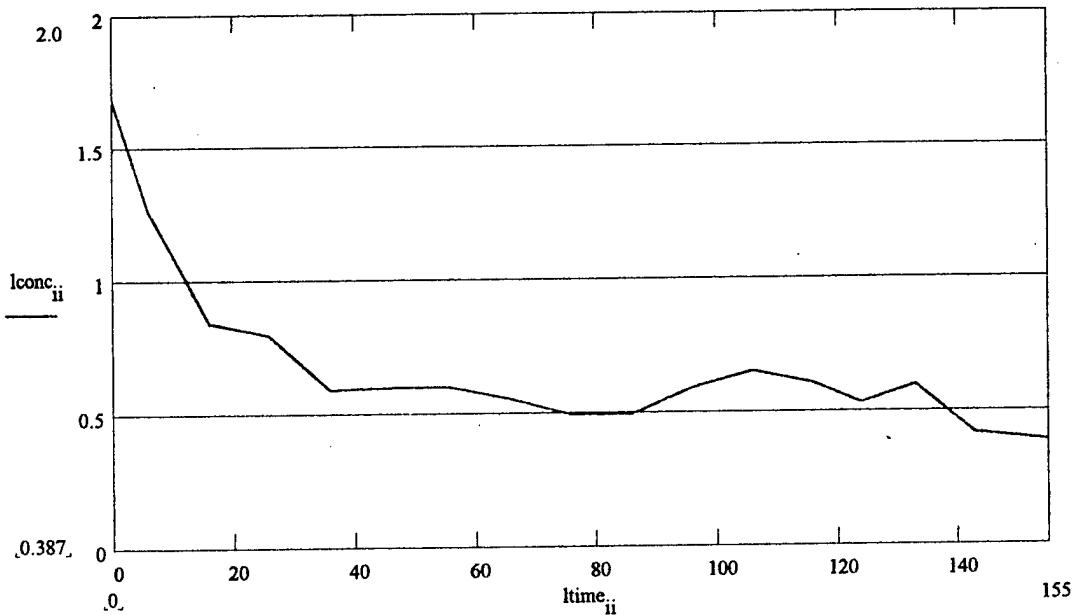


Figure . 10. Concentrations during time averaged pumping (49 m<sup>3</sup>/day).

From this simulation, the extraction well removed 13.6 percent of the mass. This is less than the higher continuous pumping rate, but more than the pulsed pumping mass removed (13.9 and 13.2 percents respectively). Figure 10 seems to indicate tailing at the extraction well at higher concentrations. With the lower rates of pumping, the tailing limitation becomes more prominent in the measurements of concentrations. This could represent an additional constraint for the pumping rate. If the pumping rate is not high

enough, the methodology may not reach necessary and sufficient optimality conditions and thus direct pumping operations to remain continuous. With this in mind, Figure 11 graphs apparent tailing levels for a range of pumping levels starting at 16.5 cubic meters per day and going up to 100 cubic meters per day.

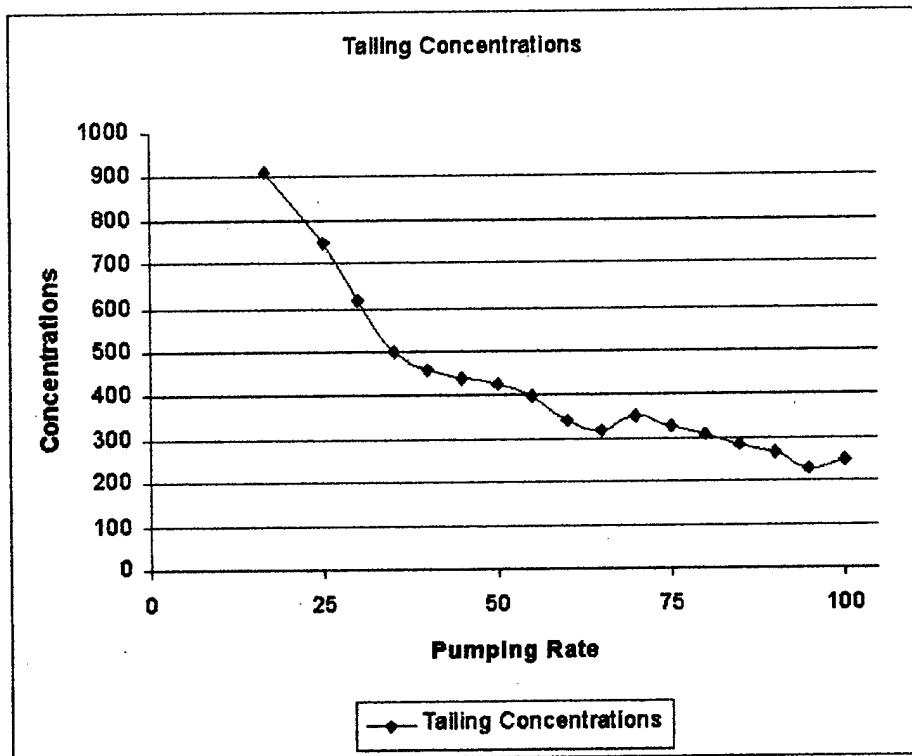


Figure 11. Apparent tailing concentrations over consistent 240 day period.

#### IV.2.2 Containment Comparisons

The simulations used a fairly uncomplicated aquifer design. In this case, containment and dewatering criteria were loose constraints. The contaminant mass downgradient of the extraction well, in all of the following cases was non-essential mass (i.e. the concentration was below the standard). In more complicated aquifer designs, these constraints would more actively participate in the overall pulsed pumping strategy. Regarding containment,

the end disposition of the contaminant plume is important aspect of comparing various methods and operations. For comparison and pumping strategy insight purposes, plume figures are provided for the pulsed pumping strategy, the continuous pumping strategy at the same rate, and the continuous pumping strategy at the lower rate.

The plume at the end of the pulsed pumping scenario is shown in Figure 12. Contours are between  $2000 \mu\text{g}/\text{m}^3$  to  $20 \mu\text{g}/\text{m}^3$ .

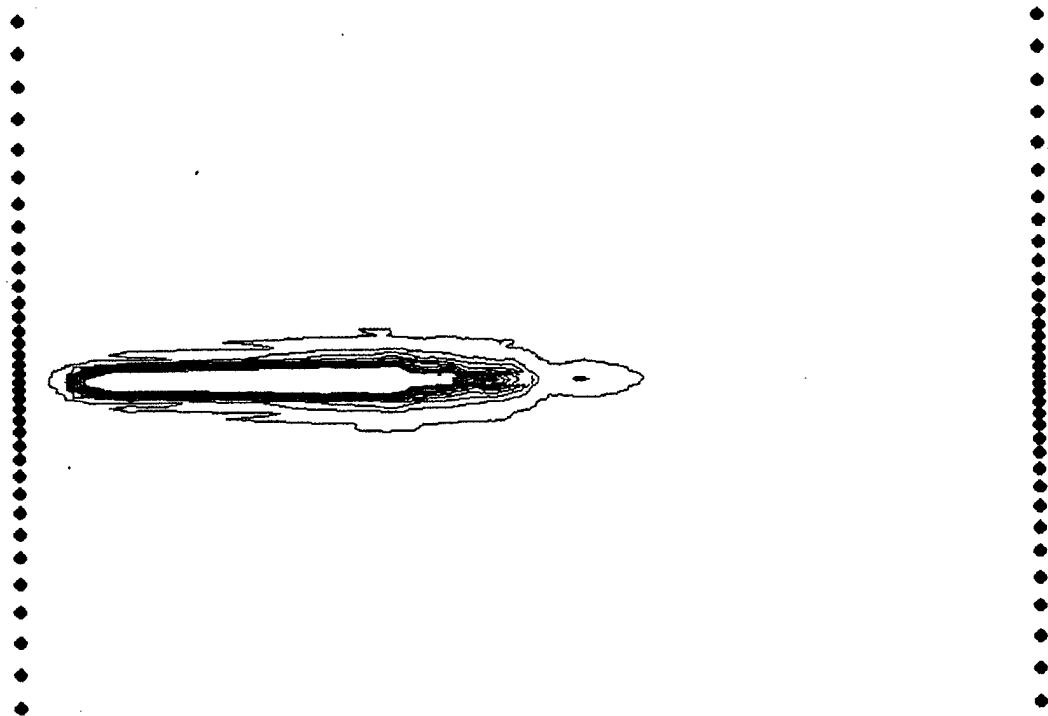


Figure . 12. Plume at the end of 575 days under pulsed pumping.

The plume at the end of continuous pumping of  $76 \text{ m}^3/\text{day}$  is shown in Figure 13. Contours are between  $2000 \mu\text{g}/\text{m}^3$  to  $20 \mu\text{g}/\text{m}^3$ .

The plume at the end of continuous pumping of  $49 \text{ m}^3/\text{day}$  is shown in Figure 14. Contours are between  $2000 \mu\text{g}/\text{m}^3$  to  $20 \mu\text{g}/\text{m}^3$ .

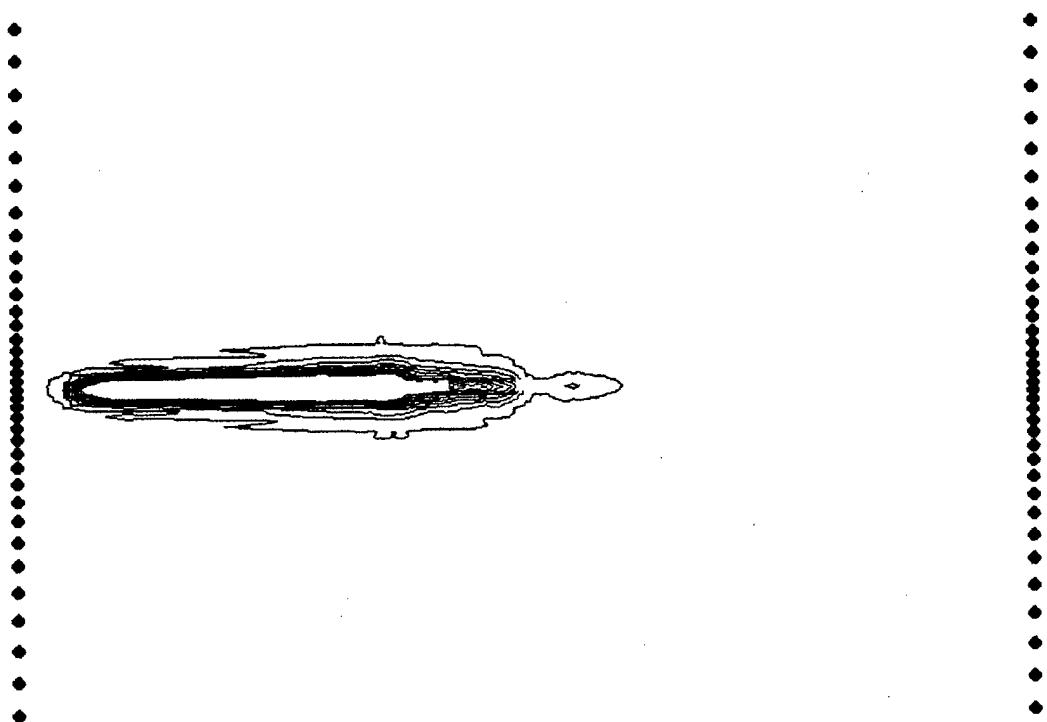


Figure . 13. Plume at the end of 575 days under continuous pumping (high).

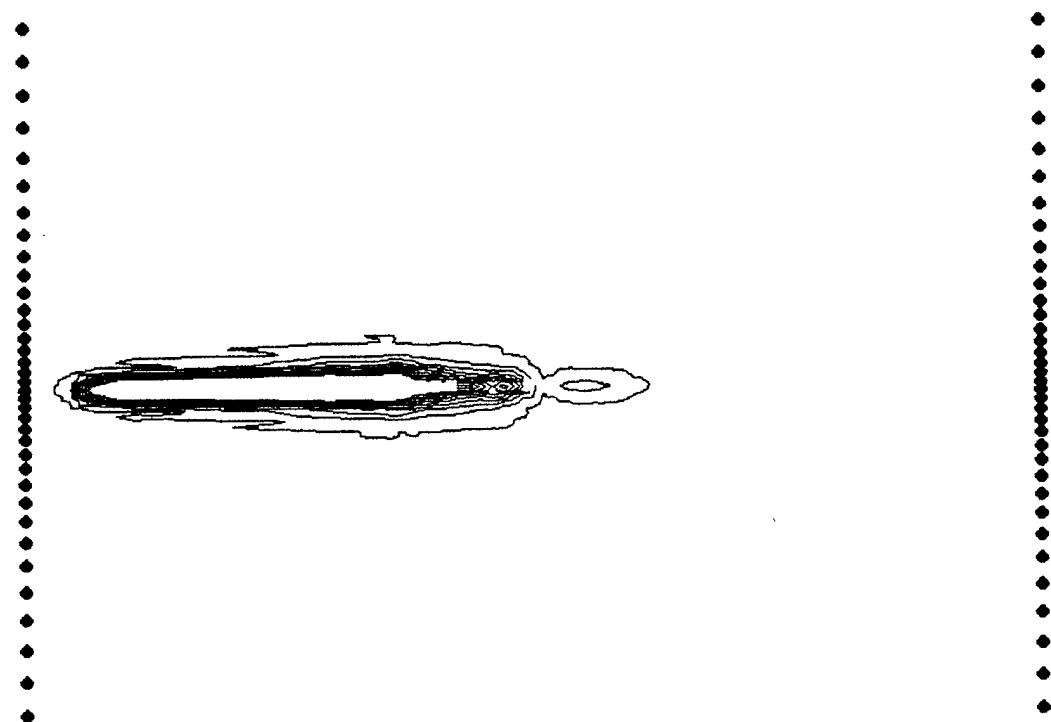


Figure . 14. Plume at end of 575 days under continuous pumping (low).

In the pulsed pumping scenario in Figure 12, the plume downgradient of the extraction well more spread out. With the constant scenario in Figure 13, the plume is much tighter. In Figure 14 with the low constant pumping rate, the plume is also tighter than the pulsed pumping scenario, but the peak concentration is higher. Again in all cases, peak downgradient concentrations were significantly lower than the standard indicating that the containment constraint was not violated.

### IV.3 Sensitivity Analysis

During the simulation, the time to  $t_1$ , the initial switching time from active to resting, was particularly important. This first time would have impact on all subsequent calculations for switching. Because of this, the sensitivity analysis focuses on the impact various parameters have on time  $t_1$ . The parameters chosen are found in the methodology, and they are the concentration scaling factor  $\sigma$ , the standard concentration  $c_s$ , the maximum pumping rate  $Q$ , and the weighting factor  $z$ . The time  $t_1$  is 50 days,  $\sigma$  is 0.021,  $c_s$  is 2000  $\mu\text{g}/\text{m}^3$ ,  $Q$  is 76  $\text{m}^3/\text{day}$ , and  $z$  is 0.999999998.

The sensitivities of  $z$  are not calculated because it is a function of  $c_s$  and there is a direct inverse relationship between the two parameters. Sensitivity is calculated using (48)

$$Sensitivity = \frac{\Delta\% \text{ in } t_1}{\Delta\% \text{ in parameter}}. \quad (48)$$

Parameter	$t_1$	Sensitivity
$\sigma +10\%$	+40%	4
$\sigma -10\%$	-48%	4.8
$c_s +10\%$	+30%	3
$c_s -10\%$	-20%	2
$Q+32\%$	-40%	-1.25
$Q-35\%$	+180%	-5.1

Table . 9. Sensitivity analysis.

## V. Conclusions and Recommendations

### V.1 Overview

Initial research revealed an enormous amount of literature on groundwater remediation. This research was approached with a determination to search out new theories in the field of optimizing pulsed pumping in an analytical, mathematical approach. Harvey et al. developed a Laplace domain Green's function solution for pumping periods and coupled it with an analytic solution for resting periods [28]. Unfortunately, their solution produces uniform pumping and resting time intervals. Lawrence Schmitt and Richard Hartman developed methodology using a calculus of variations approach to determine optimal pumping and resting time intervals for several different objectives and were not limited to uniform time periods [27], [48]. Other forms of pulsed pumping optimization methodologies could not be found. It is hoped that future interest will be spurred and that applications could be taken to the field where operations could be improved and costs reduced.

One of the primary objectives of this work is to provide a rough framework to bridge analysis with potential applications of the methodology. From this framework, further research can be pursued and lead to more robust theory. Application is one of the next logical steps that would further support the methodology and clear much of the skepticism surrounding optimized pulsed-pumping.

This research continues to support the method of pulsed pumping operations to concurrently minimize water and maximize contaminant extracted. Results support what seems intuitive about pulsed pumping in improving operational effectiveness by simply pumping when concentrations are high and resting when the concentrations are low. Many of the

earlier arguments against pulsed pumping were hampered by a paradigm that pumping periods and resting periods had to be uniform. Clearly, this research shows that these cycles are not uniform and do not have to be.

An important distinction must be made between this methodology and other optimization methodologies. This work optimizes the scheduling process alone for a given site and a given pumping rate. Comparisons between this optimal switching-time solution and a continuous time-averaged pumping rate are invalid, because the new pumping rate would provide a new and different solution for optimal switching. At some point, the pulsed pumping methodology converges to a continuous pumping solution when the pumping rate is low enough. Faced with a lower constraint of pump rates, a situation may occur when pulsed pumping operations are clearly a better choice for remediation project managers.

## **V.2 Summary of Findings**

1. This work provides a general form of the essential concentration function. Selected parabolic, third-order and fifth-order polynomial forms were analyzed for potential roots to meet necessary optimality conditions. The third-order polynomial provided the only real, positive roots. With respect to the methodology, the roots are an important factor in whether solutions are possible.
2. The root located at the standard concentration must be an odd order to satisfy the preference for concentrations lower than the standard. A singular root provided the only form of those tested that supported a pulsed pumping solution with this methodology. The presence of roots at zero in the essential concentration function also

appear to support the subsequent  $G(t)$  function having real, positive roots.

3. The contaminant mass removed per unit volume of water increased over 47 percent by using an optimized pulsed pumping strategy. This could translate into much lower operating expenses, but additional monitoring procedures may be required.
4. During some simulations when scaling factor was varied, the methodology constrained operations to switching times that were very close together. This proved to be a very difficult objective to maintain and could also be very arduous for operators constantly making pump operation changes. Concentration rise and fall quickly in responses switches in pump operations. The periods between switching points were on the order of one day and created a chatter effect in the concentrations measured at the extraction well.
5. The comprehensive objective functional focused on remediation as constrained by containment and drawdown limitations. The containment and head constraints were not restrictive in the tested scenarios. This was due to the simplicity of the contamination site and the aquifer. With more complicated scenarios, these constraints would play a more active role in the decision process.
6. The methodology is not biased to produce just pulsed pumping solutions. Given any number of constraints or physical conditions, the methodology may direct the manager to pump continuously. At low enough pumping rates, pulsed pumping becomes continuous pumping.
7. The methodology has great potential for application, because the experiment did not

require detailed plume boundaries, source locations, or release histories in order to manage the operation. This could potentially reduce much of the site investigation costs that typically occur at remediation sites.

### **V.3 Limitations**

One limitation of this work is a lack of verification against an actual site. This work developed a hypothetical model for carrying out simulations to test the optimized pulsed pumping methodology. A test site would provide more information about applying the methodology and its advantages and limitations.

Another limitation with the model are the hydrological parameters used within the simulation. Unfortunately, the code does not include rate-limited sorption features within the transport code, but it uses local equilibrium assumptions. If rate-limited sorption was intrinsic to the model, the results would be a better depiction of reality. Heterogeneity would also be easier to incorporate for a more complicated version of the contamination problem. The aquifer model used in this research was a simple, two-dimensional model with minor heterogeneities. This situation in the field almost never occurs. The regional influences within the model were also very simple and uniform and included artificial boundaries. Added complexity would greatly enhance the robustness of the concept and give the theory more credibility.

The methodology is highly sensitive to variations of the essential concentration function. The methodology has focused on determining what form the function should take in order to provide non-trivial answers to the optimization question. The essential concentra-

tion function definition provides general guidelines for its form, but it would benefit from a stronger physical basis for specific behavior and form.

Pump-and-treat technology is no longer considered an adequate remediation technology by itself at most real-world sites. The most appropriate application is in maintaining hydraulic control. This work would benefit from creative ideas that would aggregate this technique with other remediation strategies to develop a synergistic strategy for remediation.

#### **V.4 Recommendations**

The recommendations for this research are primarily focused on eliminating the limitations mentioned earlier.

1. Reaccomplish the simulations using a transport code that incorporates rate-limited sorptions characteristics. This would allow a researcher to investigate and develop heterogeneities that are more suitable to field applications. The behavior of the contaminant would be more realistic at a finer scale, and probably produce better realizations of contaminant concentration at given points. The Army Waterways Experiment Station has stated that GMS 3.0 will be released in the summer of 1999 that includes a the graphical interface MT3DMS, which can model rate-limited sorption.
2. The analytical approach taken in this thesis could have some interesting applications in other approaches to remediation. For example, in-situ bioremediation may benefit from optimal pulsed nutrient injection by looking at pumping rates and nutrients concentrations as input parameters and bacterial concentrations as feedback

parameters.

3. In further numerical modeling, more complexity is definitely required. A larger scale that includes a greater number of influences would add more realism. Additional wells, areal recharge, rivers, lakes, numerous contamination sources, and aquifer stratifications are some of the potential additions that would yield more useful information. Additional extraction wells working in concert and also some injection wells might provide interesting results.
4. There are still some assumptions within the optimization methodology that require analytical solutions. Particularly, the first time derivative of the concentration at the extraction well needs a functions that can obviate the need for a numerical approximation.
5. The essential concentration function requires further analysis and development of the physical basis. Other forms need to be tested and evaluated.
6. A existing remediation site with a fully developed plume footprint and history would be an excellent candidate for application.

## APPENDIX A Capture Zone Calculations

Calculations for capture zone regions as found in Fetter, 1994.

Transmissivity (m<sup>2</sup>/day)  $T = 124.4$

Regional Hydraulic Gradient  $i = 0.01$

Pumping Rate (m<sup>3</sup>/day)  $Q = 200$

Capture Zone

$$f(y) = \frac{-y}{\tan(2\pi Ti \frac{y}{Q})}$$

Max Capture Width (half)

$$y_{\max} = \frac{-Q}{2Ti} = 80.386$$

Stagnation Point

$$x_{stag} = \frac{-Q}{2\pi Ti} = 25.588$$

Within the thesis simulation, this pumping rate is excessive considering the plume dimensions. Therefore, a lower pumping rate should be used. See the next calculations.

Now for a more optimal pumping rate, given the plume characteristics from the thesis simulation. Plume dimensions at 10 meters upgradient from the extraction well were 20 meters above the bisect.

Pumping Rate (m<sup>3</sup>/day)  $Q_{new} = -76$

Capture Zone

Max Capture Width (half)  $y_{\max} = 30.547$

Stagnation Point  $x_{stag} = 9.723$

Starting at day 665, the pumping rate needed to contain the plume will be 76 m<sup>3</sup>/day.

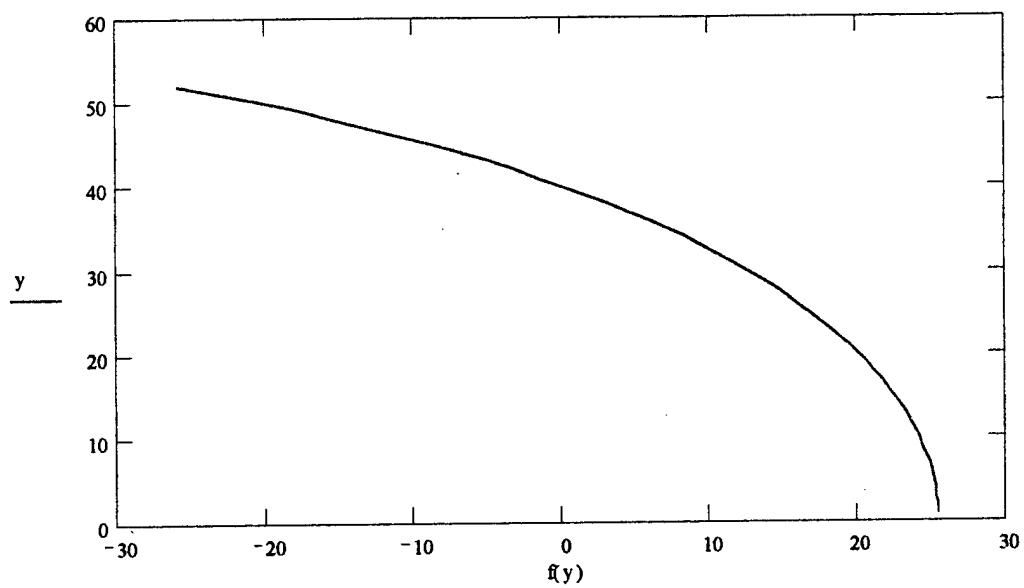


Figure . A-1. Capture zone for 200 cubic meters per day pumping rate.

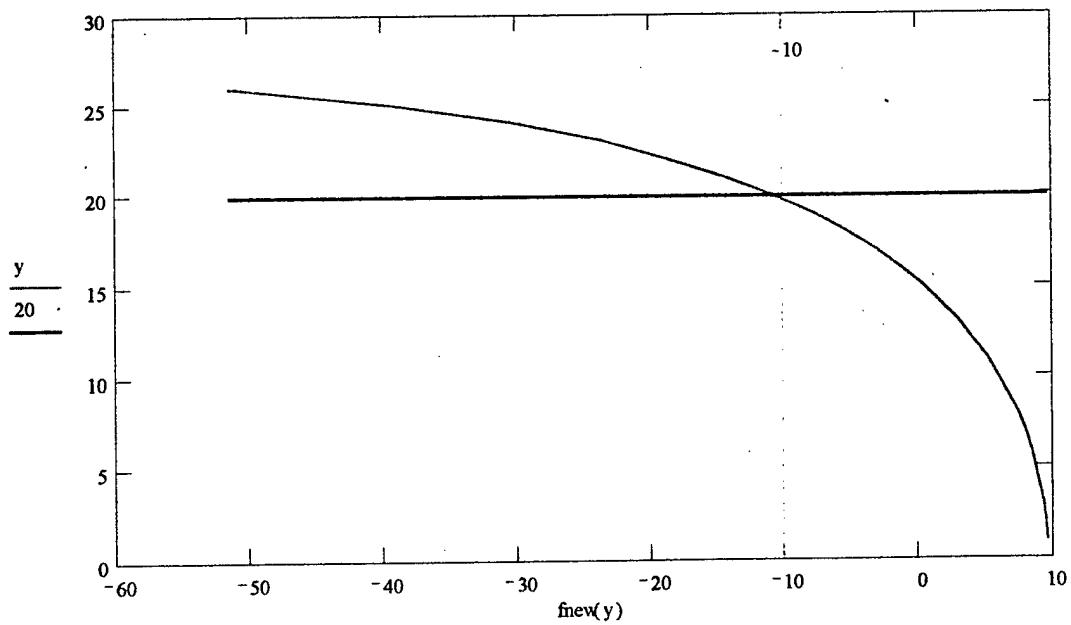


Figure . A-2. Capture zone for 76 cubic meters per day pumping rate.

Now for the reduced continuous pumping rate that is equivalent to the pulsed pumping rate over a time average.

Pumping Rate (m<sup>3</sup>/day)  $Q = -49$

Capture Zone

Max Capture Width (half)  $y_{max} = 20.016$

Stagnation Point  $x_{stag} = 6.371$

At the pumping rate of 49 m<sup>3</sup>/day, the capture zone is 14 m from the bisect at a point 10 m upgradient of the extraction well. With a monitoring well at 7 m downgradient, the location is outside the capture zone and direct influence.

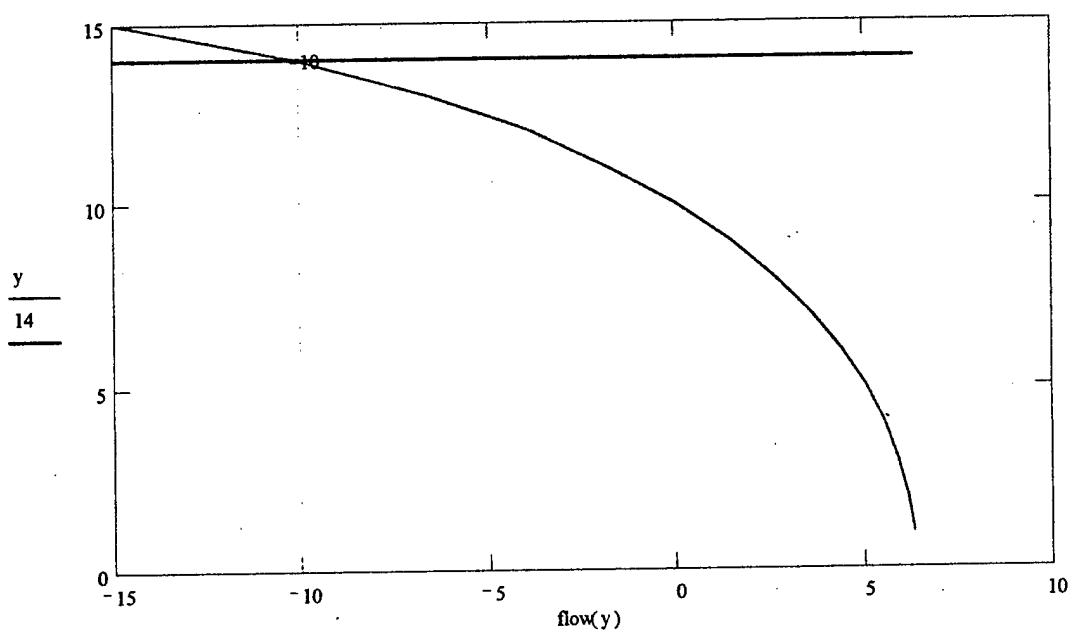


Figure . A-3. Capture zone for 49 cubic meters per day pumping rate.

## APPENDIX B Example 1 Study and Simulation Results

The following file contains excerpts from the original MATHCAD 7 spreadsheet document. The concentration figures are from measurements at the extraction well and a monitoring point located down-gradient from the extraction well. The file also contains the functional  $G(t)$  that uses the concentration data to produce the optimal transition point for the extraction well operation.

The weighting balances 2000  $\mu\text{g}$  with 1 cubic meter.

Weighting Factor is  $z = 0.999999998$ .

Water Density in  $\mu\text{g}/\text{m}^3$  is  $\rho_w = 10^{12}$ .

The solute used in this simulation is carbon tetrachloride. Typical concentrations found in contaminated groundwater are about 5  $\mu\text{g}/\text{L}$ . Under World Health Organization (WHO) the risk-based standard for carbon tetrachloride is 2  $\mu\text{g}/\text{L}$ , which will be used to demonstrate this methodology.

Concentration Standard in  $\mu\text{g}/\text{m}^3$  is  $c_s = 2000$ . This is the same as 2.0 ppb.

The scaling factor is chosen to satisfy requirements for the objective function, which needs two real, positive roots. The scaling factor, 0.021 provides roots at concentrations 439 and 851  $\text{mg}/\text{m}^3$ .

Concentration Scaling Factor in  $\text{m}^3/\mu\text{g}$  is  $\sigma = 0.021$ .

Coefficients for the  $G(t)$  function.

$K_i$	Formula	Value
$K_0$	$(z - 1)\rho_w$	$-2 * 10^3$
$K_1$	0	0
$K_2$	$-z\sigma c_s$	-42
$K_3$	$z$	0.999999998

The function  $G(t)$  takes concentration readings at specific times from the extraction well, so the following function  $G(c)$  is the same as long as the concentrations are ordered.

$$G(t) = K_0 - K_2(\sigma c)^2 - 2K_3(\sigma c)^3$$

The roots were determined to be (-6.077, 9.209, 17.868) and are unitless. The positive roots correspond to concentrations  $439 \mu\text{g}/\text{m}^3$  and  $851 \mu\text{g}/\text{m}^3$  respectively. The roots are evident in Figure B-1.

Figure B-2 is a plot of  $G(t)$  for 155 days, under pulsed pumping.

Figure B-3 represents a time series plot of concentration at the extraction well.

Figure B-4 represents a time series plot of concentration at extraction well under continual pumping at 76 cubic meters per day.

Figure B-5 represents a time series plot of concentration at the extraction well under continual pumping at 49 cubic meters per day.

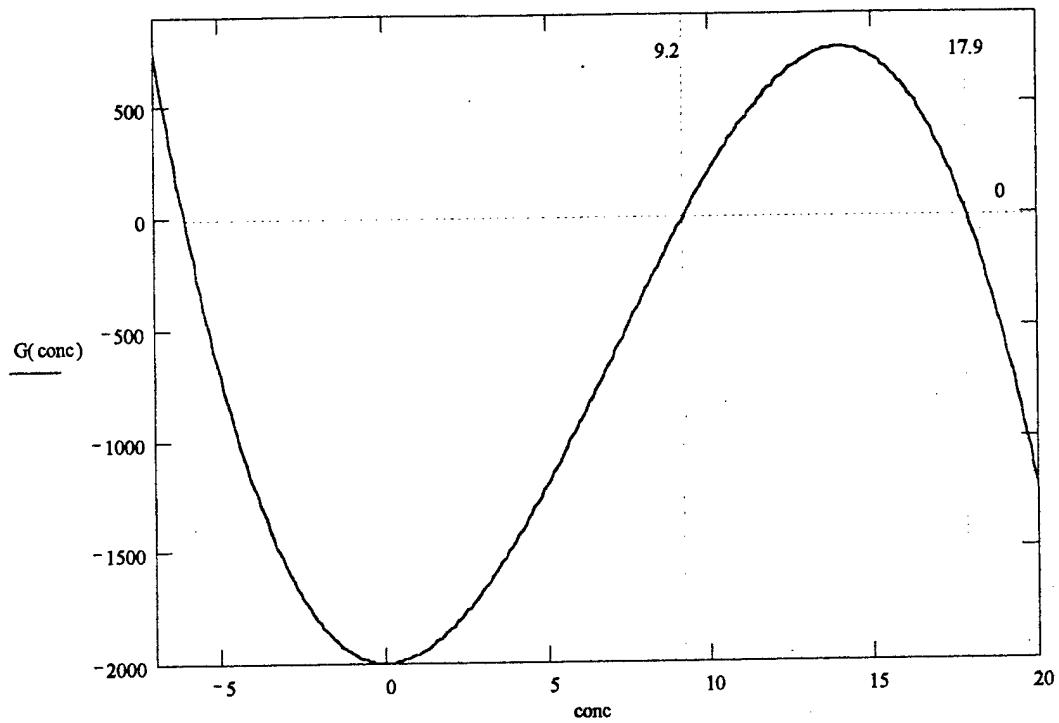


Figure . B-1. Plot of  $G(c)$  for a range of scaled concentrations

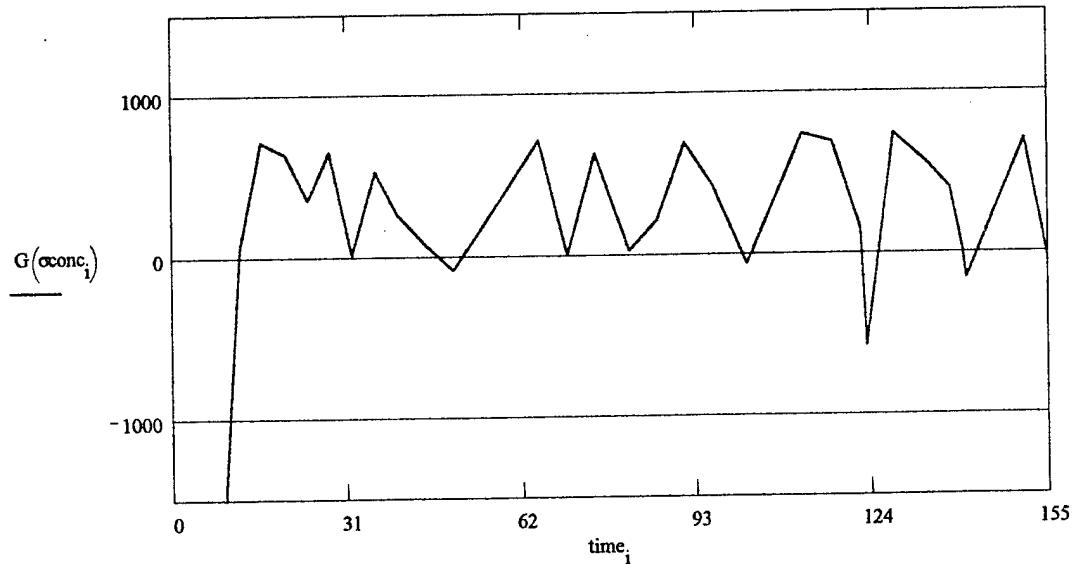


Figure . B-2. Time series of  $G(t)$

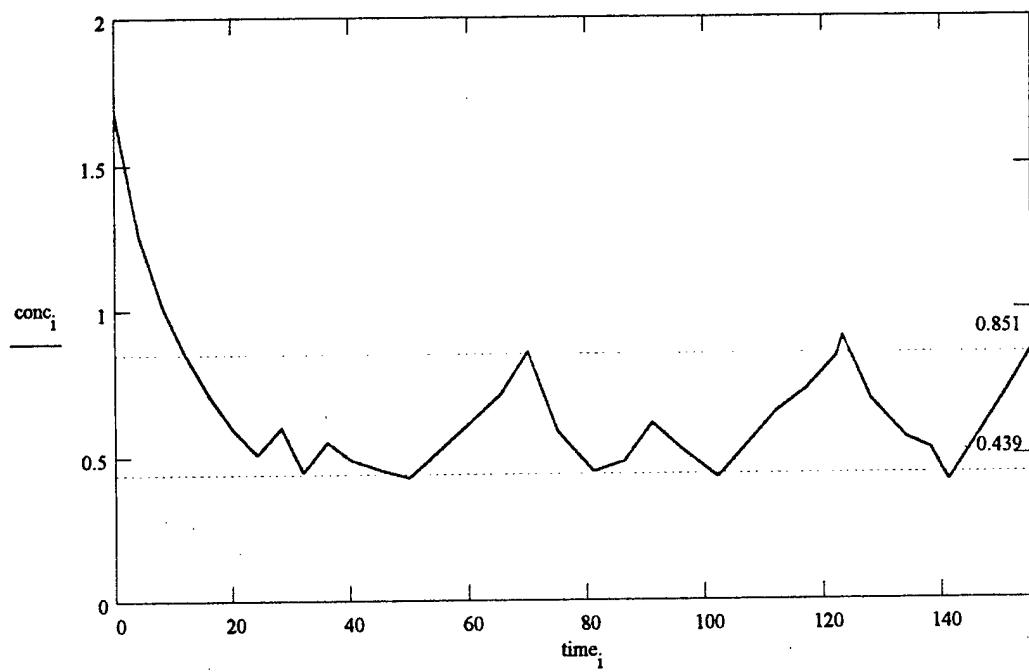


Figure . B-3. Concentrations at extraction well under pulsed pumping

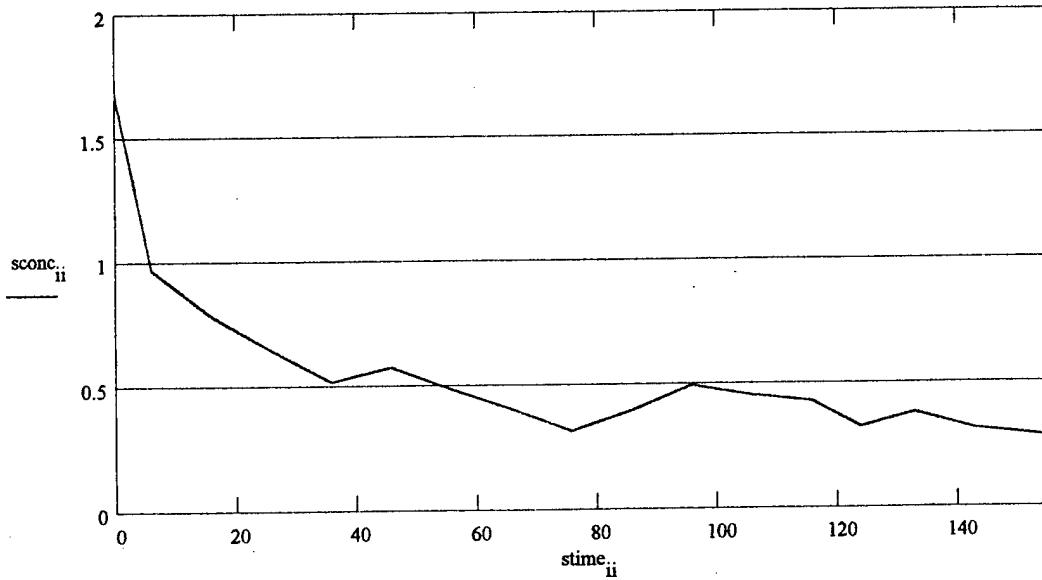


Figure . B-4. Concentrations at extraction well under continuous pumping of 76

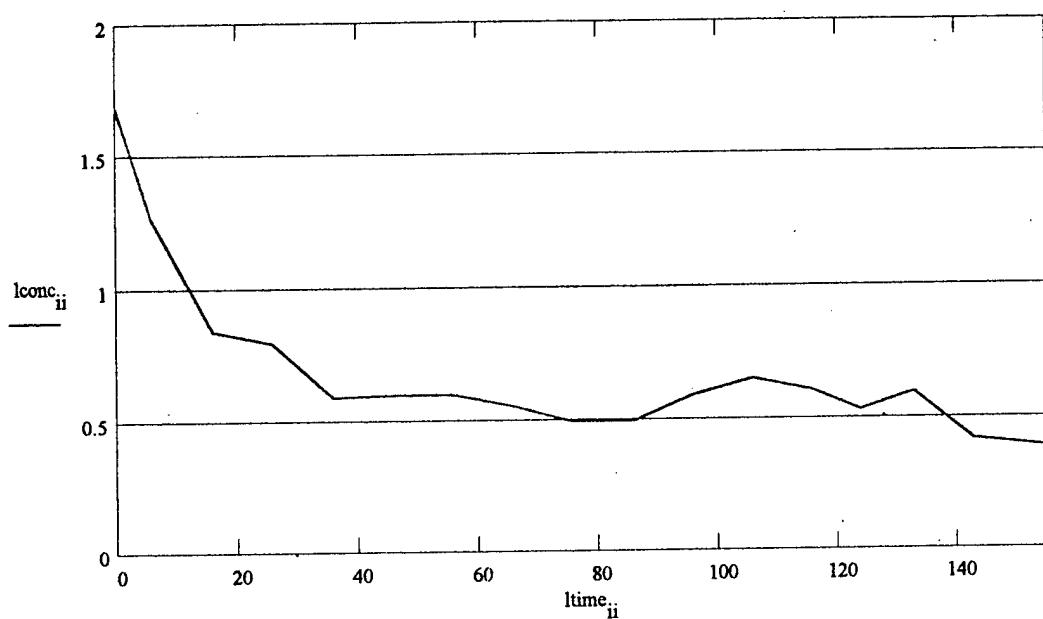


Figure . B-5. Concentrations at extraction well under continuous pumping 49.

## APPENDIX C Example 2 Study - Fifth-Order Polynomial

The following MATHCAD 7 spreadsheet presents the results from analyzing a fifth-order polynomial as an essential concentration function. A plot will display the function over a range of concentrations.

Weighting Factor is  $z = 0.999999998$ .

Water Density in  $\mu\text{g}/\text{m}^3$  is  $\rho_w = 10^{12}$ .

Concentration Standard in  $\mu\text{g}/\text{m}^3$  is  $c_s = 2000$ .

Concentration Scaling Factor in  $\text{m}^3/\mu\text{g}$  is  $\sigma = 0.005$ .

The coefficients for the optimization function are now

Coefficient	Formula	Value
$K_0$	$(z - 1)\rho_w - \sigma^5 c_s^5 z$	$-1.002 * 10^5$
$K_1$	0	0
$K_2$	$\sigma^3 c_s^3 z$	$-1 * 10^3$
$K_3$	$\sigma^2 c_s^2 z$	100
$K_4$	$\sigma c_s z$	10
$K_5$	$z$	0.999999998

The function  $G(t)$  has the form.

$$G(t) = K_0 - 10K_2(\sigma c)^2 - 20K_3(\sigma c)^3 - 15K_4(\sigma c)^4 - 4K_5(\sigma c)^5$$

Roots are

$$(-2.502, 9.003 \pm 1.043i, 10.998 \pm 0.963i).$$

The plotted response over a range of values is shown in Figure C-1.

Unfortunately, the only real root is negative. Varying the value of the scaling factor,  $\sigma$ , yielded similar results.

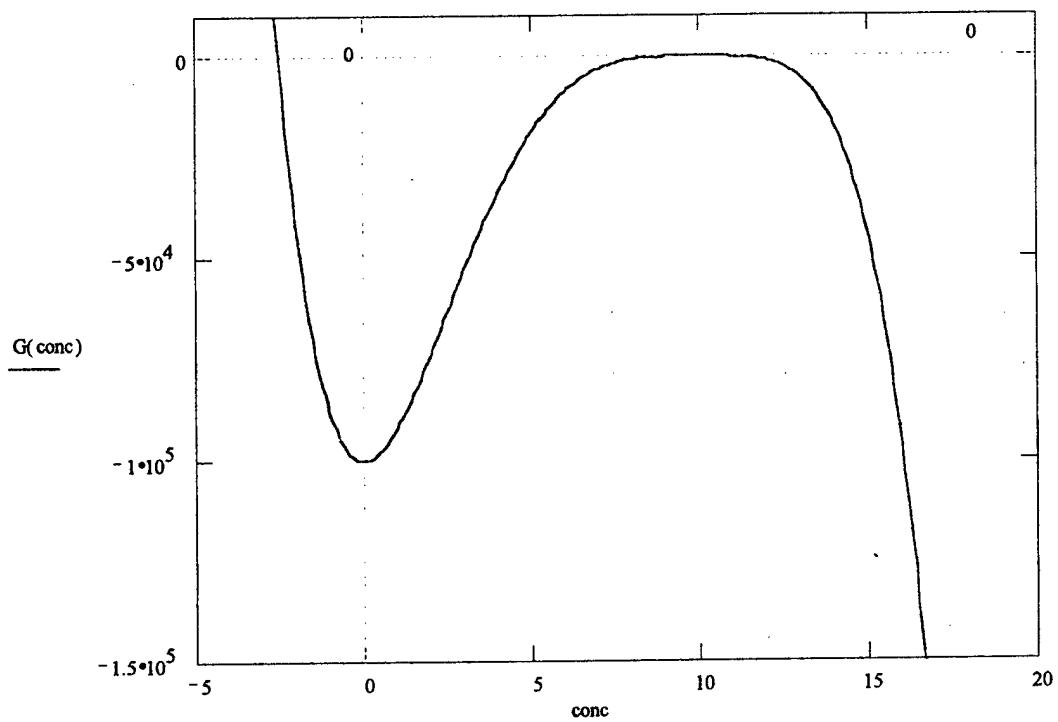


Figure . C-1. Fifth-order polynomial response.

## APPENDIX D Example 3 Study - Parabolic

The following MATHCAD 7 spreadsheet presents the results from analyzing a second-order polynomial as an essential concentration function. A plot will display the function over a range of concentrations.

Weighting Factor is  $z = 0.999999998$ .

Water Density in  $\mu\text{g}/\text{m}^3$  is  $\rho_w = 10^{12}$ .

Concentration Standard in  $\mu\text{g}/\text{m}^3$  is  $c_s = 2000$ .

Concentration Scaling Factor in  $\text{m}^3/\mu\text{g}$  is  $\sigma = 0.12$ .

The function  $G(t)$  has the form.

$$G(t) = (z - 1)\rho_w + z\sigma^2 c_s^2 - z(\sigma c)^2$$

Over a range of concentrations, the plot of  $G(c)$  is observable in Figure D-1.

The positive root corresponds a concentration of  $1997 \mu\text{g}/\text{m}^3$ , which is just below the standard concentration. If this becomes the choice for an essential concentration function, the operator would be unable to reach sufficient optimality conditions and would continuously pump. Various scaling values were used with similar results.

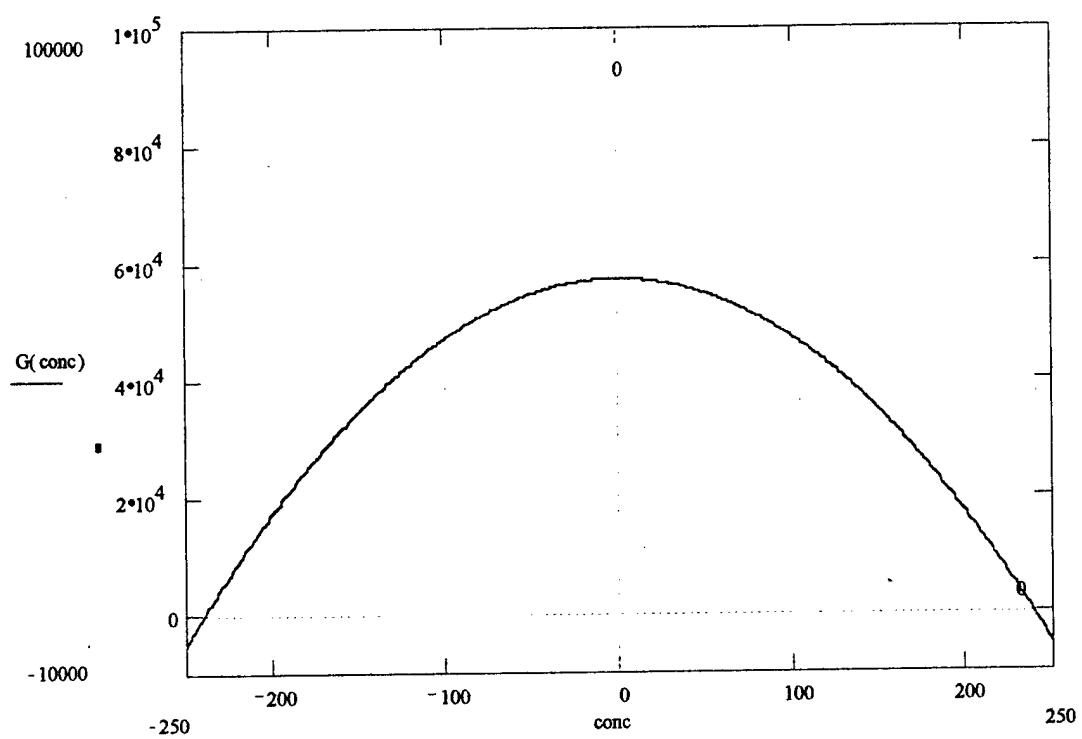


Figure . D-1. Response of parabolic function.

## APPENDIX E Output File Excerpts

### E.1 MODFLOW File

1 U.S.G.S. MODULAR FINITE-DIFFERENCE GROUND-WATER MODEL

0Thesis Stage 1 Tay W. Johannes 16 Jan 99

1 LAYERS 37 ROWS 43 COLUMNS

10 STRESS PERIOD(S) IN SIMULATION

MODEL TIME UNIT IS DAYS

0I/O UNITS:

ELEM OF IUNIT: 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

I/O UNIT: 11 13 0 0 0 0 0 12 0 0 10 0 0 0 0 0 0 0 0 29 0 0

0BAS1 – BASIC MODEL PACKAGE, VRS 1, 9/1/87 INPUT READ FROM UNIT 1

ARRAYS RHS AND BUFF WILL SHARE MEMORY.

START HEAD NOT SAVED – DRAWDOWN CANNOT BE CALCULATED

12812 ELEMENTS IN X ARRAY ARE USED BY BAS

12812 ELEMENTS OF X ARRAY USED OUT OF 9000000

0BCF3 – BLOCK-CENTERED FLOW PACKAGE, VERSION 3, 7/9/92 INPUT

READ FROM UNIT 11

TRANSIENT SIMULATION

CELL-BY-CELL FLOWS WILL BE RECORDED ON UNIT 40

HEAD AT CELLS THAT CONVERT TO DRY= -888.00

WETTING CAPABILITY IS NOT ACTIVE

LAYER AQUIFER TYPE INTERBLOCK T

---

100-HARMONIC

1592 ELEMENTS IN X ARRAY ARE USED BY BCF

14404 ELEMENTS OF X ARRAY USED OUT OF 9000000

0WEL1 - WELL PACKAGE, VERSION 1, 9/1/87 INPUT READ FROM 13

MAXIMUM OF 14 WELLS

CELL-BY-CELL FLOWS WILL BE RECORDED ON UNIT 40

56 ELEMENTS IN X ARRAY ARE USED FOR WELLS

14460 ELEMENTS OF X ARRAY USED OUT OF 9000000

0SIP1 - STRONGLY IMPLICIT PROCEDURE SOLUTION PACKAGE, VERSION

1, 9/1/87

INPUT READ FROM UNIT 12

MAXIMUM OF 50 ITERATIONS ALLOWED FOR CLOSURE

5 ITERATION PARAMETERS

6569 ELEMENTS IN X ARRAY ARE USED BY SIP

21029 ELEMENTS OF X ARRAY USED OUT OF 9000000

1Thesis Stage 1 Tay W. Johannes 16 Jan 99

0

BOUNDARY ARRAY FOR LAYER 1 WILL BE READ ON UNIT 1 USING FOR-  
MAT: (43I3)

---

1 2 3 4 5 6 7 8 9 10

11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43							

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0AQUIFER HEAD WILL BE SET TO -999.00 AT ALL NO-FLOW NODES (IBOUND=0).

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INITIAL HEAD FOR LAYER 1 WILL BE READ ON UNIT 1 USING FORMAT:

(10G15.6)

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0HEAD PRINT FORMAT IS FORMAT NUMBER 0 DRAWDOWN PRINT FOR-

MAT IS FORMAT NUMBER 0

0HEADS WILL BE SAVED ON UNIT 30 DRAWDOWNS WILL BE SAVED ON  
UNIT 35

0OUTPUT CONTROL IS SPECIFIED EVERY TIME STEP

0 COLUMN TO ROW ANISOTROPY = 1.000000

0

DELR WILL BE READ ON UNIT 11 USING FORMAT: (10G15.6)

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0

DELC WILL BE READ ON UNIT 11 USING FORMAT: (10G15.6)

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0 PRIMARY STORAGE COEF = 0.5000000E-04 FOR LAYER 1

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TRANSMIS. ALONG ROWS FOR LAYER 1 WILL BE READ ON UNIT 11 USING  
FORMAT: (10G15.6)

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SOLUTION BY THE STRONGLY IMPLICIT PROCEDURE

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0 MAXIMUM ITERATIONS ALLOWED FOR CLOSURE = 50

ACCELERATION PARAMETER = 1.0000

HEAD CHANGE CRITERION FOR CLOSURE = 0.10000E-02

SIP HEAD CHANGE PRINTOUT INTERVAL = 999

0 CALCULATE ITERATION PARAMETERS FROM MODEL CALCULATED WSEED

1 STRESS PERIOD NO. 1, LENGTH = 100.0000

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NUMBER OF TIME STEPS = 10

MULTIPLIER FOR DELT = 1.000

INITIAL TIME STEP SIZE = 10.00000

0 14 WELLS

LAYER ROW COL STRESS RATE WELL NO.

---

1 19 22 0.0000 1

1 19 14 5.0000 2

1 19 13 5.5000 3

1 19 12 6.0000 4

1 19 11 6.6000 5

1 19 10 7.3000 6

1 19 8 8.6400 7

1 19 9 8.6400 8

1 19 15 8.6400 9

1 19 6 8.6400 10

1 19 5 8.6400 11

1 19 4 8.6400 12

1 19 3 8.6400 13

1 19 7 8.6400 14

0AVERAGE SEED = 0.00074996

MINIMUM SEED = 0.00000018

0

5 ITERATION PARAMETERS CALCULATED FROM AVERAGE SEED:

0.0000000E+00 0.8345147E+00 0.9726146E+00 0.9954681E+00 0.9992501E+00

0

17 ITERATIONS FOR TIME STEP 1 IN STRESS PERIOD 1

0HEAD/DRAWDOWN PRINTOUT FLAG = 1 TOTAL BUDGET PRINTOUT FLAG

= 1 CELL-BY-CELL FLOW TERM FLAG = 1

0OUTPUT FLAGS FOR ALL LAYERS ARE THE SAME:

HEAD DRAWDOWN HEAD DRAWDOWN

PRINTOUT PRINTOUT SAVE SAVE

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0 0 1 0

“ STORAGE“ BUDGET VALUES WILL BE SAVED ON UNIT 40 AT END OF TIME STEP 1, STRESS PERIOD 1

“ CONSTANT HEAD“ BUDGET VALUES WILL BE SAVED ON UNIT 40 AT END OF TIME STEP 1, STRESS PERIOD 1

“ FLOW RIGHT FACE “ BUDGET VALUES WILL BE SAVED ON UNIT 40 AT END OF TIME STEP 1, STRESS PERIOD 1

“ FLOW FRONT FACE “ BUDGET VALUES WILL BE SAVED ON UNIT 40 AT END OF TIME STEP 1, STRESS PERIOD 1

“ WELLS“ BUDGET VALUES WILL BE SAVED ON UNIT 40 AT END OF TIME STEP 1, STRESS PERIOD 1

HEADS AND FLOW TERMS SAVED ON UNIT 29 FOR USE BY MT3D TRANS-  
PORT MODEL

0HEAD WILL BE SAVED ON UNIT 30 AT END OF TIME STEP 1, STRESS PE-  
RIOD 1

0

VOLUMETRIC BUDGET FOR ENTIRE MODEL AT END OF TIME STEP 1 IN  
STRESS PERIOD 1

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0 CUMULATIVE VOLUMES  $L^3$       RATES FOR THIS TIME STEP  $L^3/T$

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IN:

STORAGE = 0.0000

IN:

STORAGE = 0.0000

CONSTANT HEAD = 1612.3

WELLS = 995.20

0 TOTAL IN = 2607.5

0 OUT:

STORAGE = 0.43509

CONSTANT HEAD = 2598.0

WELLS = 0.0000

0 TOTAL OUT = 2598.4

0 IN - OUT = 9.1353

0 PERCENT DISCREPANCY = 0.35

CONSTANT HEAD = 161.23

WELLS = 99.520

TOTAL IN = 260.75

OUT:

STORAGE = 0.43509E-01

CONSTANT HEAD = 259.80

WELLS = 0.0000

TOTAL OUT = 259.84

IN - OUT = 0.91354

PERCENT DISCREPANCY = 0.35

VOLUMETRIC BUDGET FOR ENTIRE MODEL AT END OF TIME STEP 2 IN  
STRESS PERIOD 10

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0 CUMULATIVE VOLUMES L<sup>3</sup>

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RATES FOR THIS TIME STEP L<sup>3</sup>/T

IN:

STORAGE = 1.9134

CONSTANT HEAD = 0.13708E+06

WELLS = 9952.0

0 TOTAL IN = 0.14703E+06

0 OUT:

STORAGE = 1.9084

IN:

STORAGE = 0.62864E-05

CONSTANT HEAD = 233.14

WELLS = 0.0000

TOTAL IN = 233.14

OUT:

STORAGE = 0.86199E-05

CONSTANT HEAD = 0.11998E+06	CONSTANT HEAD = 232.62
WELLS = 27068.	WELLS = 0.0000
0 TOTAL OUT = 0.14705E+06	TOTAL OUT = 232.62
0 IN - OUT = -19.078	IN - OUT = 0.51973
0 PERCENT DISCREPANCY = -0.01	PERCENT DISCREPANCY = 0.22

## E.2 MT3D File

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+++++
+++
+ M T 3 D +
+ A Modular Three-Dimensional Transport Model +
+ For Simulation of Advection, Dispersion and Chemical Reactions +
+ of Contaminants in Groundwater Systems +
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| M T | Thesis Stage II

| 3 D | Tay W. Johannes 9 Feb 99

---

THE TRANSPORT MODEL CONSISTS OF 1 LAYER(S) 37 ROW(S) 43 COL-  
UMN(S)

NUMBER OF STRESS PERIOD(S) IN SIMULATION = 10

UNIT FOR TIME IS days UNIT FOR LENGTH IS m UNIT FOR MASS IS mg

MAJOR TRANSPORT COMPONENTS TO BE SIMULATED:

1 ADVECTION

2 DISPERSION

3 SINK AND SOURCE MIXING

4 CHEMICAL REACTIONS (DECAY AND/OR SORPTION)

BTN1 – BASIC TRANSPORT PACKAGE, VER DOD\_1.5, JULY 1996, INPUT READ

FROM UNIT 1

19252 ELEMENTS OF THE X ARRAY USED BY THE BTN PACKAGE

1592 ELEMENTS OF THE IX ARRAY USED BY THE BTN PACKAGE

ADV1 – ADVECTION PACKAGE, VER DOD\_1.5, JULY 1996, INPUT READ FROM

UNIT 2

ADVECTION IS SOLVED WITH THE HYBRID [MOC]/[MMOC] SCHEME

COURANT NUMBER ALLOWED IN SOLVING THE ADVECTION TERM = 1.50

MAXIMUM NUMBER OF MOVING PARTICLES ALLOWED = 75000

300000 ELEMENTS OF THE X ARRAY USED BY THE ADV PACKAGE

1591 ELEMENTS OF THE IX ARRAY USED BY THE ADV PACKAGE

DSP1 – DISPERSION PACKAGE, VER DOD\_1.5, JULY 1996, INPUT READ FROM

UNIT 3

7958 ELEMENTS OF THE X ARRAY USED BY THE DSP PACKAGE

0 ELEMENTS OF THE IX ARRAY USED BY THE DSP PACKAGE

SSM1 – SINK & SOURCE MIXING PACKAGE, VER DOD\_1.5, JULY 1996, IN-

PUT READ FROM UNIT 4

MAJOR STRESS COMPONENTS PRESENT IN THE FLOW MODEL:

1 WELL

MAXIMUM NUMBER OF POINT SINKS/SOURCES = 88

528 ELEMENTS OF THE X ARRAY USED BY THE SSM PACKAGE

0 ELEMENTS OF THE IX ARRAY BY THE SSM PACKAGE

RCT1 - CHEMICAL REACTIONS PACKAGE, VER DOD\_1.5, JULY 1996, INPUT

READ FROM UNIT 9

TYPE OF SORPTION SELECTED IS [LINEAR]

NO FIRST-ORDER RATE REACTION IS SIMULATED

3 ELEMENTS OF THE X ARRAY USED BY THE RCT PACKAGE

0 ELEMENTS OF THE IX ARRAY USED BY THE RCT PACKAGE

.....  
327742 ELEMENTS OF THE X ARRAY USED OUT OF 3000000

3184 ELEMENTS OF THE IX ARRAY USED OUT OF 300000

.....  
LAYER NUMBER AQUIFER TYPE

1 0

WIDTH ALONG ROWS (DELR) READ ON UNIT 1 USING FORMAT: "(10G15.6)"

1 2 3 4 5 6 7 8 9 10  
11 12 13 14 15 16 17 18 19 20

21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43							

.....

1 11.23 11.23 11.23 11.12 10.11 9.190 8.354 7.595 6.905 6.277  
 5.706 5.187 4.716 4.287 3.897 3.543 3.221 2.928 2.662 2.420  
 2.200 2.000 2.200 2.420 2.662 2.928 3.221 3.543 3.897 4.287  
 4.716 5.187 5.706 6.277 6.905 7.595 8.354 9.190 10.11 11.12  
 11.89 11.89 11.89

WIDTH ALONG COLS (DELC) READ ON UNIT 1 USING FORMAT: "(10G15.6)"

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1	2	3	4	5	6	7	8	9	10
11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
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 2.420 2.662 2.928 3.221 3.543 3.897 4.287 4.716 5.187 5.706  
 6.277 6.905 7.595 8.114 8.114 8.114 8.114

TOP ELEV. OF 1ST LAYER = 20.00000

CELL THICKNESS (DZ) = 20.00000 FOR LAYER 1

EFFECTIVE POROSITY FOR LAYER 1 READ ON UNIT 1 USING FORMAT: “  
(10G15.6)“

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1	2	3	4	5	6	7	8	9	10
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21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43							

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CONCN. BOUNDARY ARRAY = 1 FOR LAYER 1

INITIAL CONCENTRATION = 0.000000 FOR LAYER 1

VALUE INDICATING INACTIVE CONCENTRATION CELLS = -999.0000

## OUTPUT CONTROL OPTIONS

---

PRINT CELL CONCENTRATION USING FORMAT CODE: 1

PRINT PARTICLE NUMBER IN EACH CELL USING FORMAT CODE: 1

PRINT RETARDATION FACTOR USING FORMAT CODE: 1

PRINT DISPERSION COEFFICIENT USING FORMAT CODE: 1

SAVE CONCENTRATION IN UNFORMATTED FILE [MT3D.\_UCN] ON UNIT 18

SIMULATION RESULTS ARE SAVED EVERY 2 TRANSPORT STEP(S)

NUMBER OF OBSERVATION POINTS = 0

A ONE-LINE SUMMRY OF MASS BALANCE FOR EACH STEP SAVED IN FILE

[MT3D.MAS] ON UNIT 19

MAXIMUM LENGTH ALONG THE X (J) AXIS = 272.0000

MAXIMUM LENGTH ALONG THE Y (I) AXIS = 190.0000

MAXIMUM LENGTH ALONG THE Z (K) AXIS = 20.00000

## ADVECTION SOLUTION OPTIONS

---

METHOD FOR PARTICLE TRACKING IS [4TH ORDER]

CONCENTRATION WEIGHTING FACTOR = 0.500

THE CONCENTRATION GRADIENT CONSIDERED NEGLIGIBLE [DCEPS] =

0.1000000E-04

INITIAL PARTICLES ARE PLACED RANDOMLY WITHIN CELL BLOCK

PARTICLE NUMBER PER CELL IF DCCELL =< DCEPS = 0

PARTICLE NUMBER PER CELL IF DCCELL > DCEPS = 16

MINIMUM PARTICLE NUMBER ALLOWD PER CELL = 2

MAXIMUM PARTICLE NUMBER ALLOWD PER CELL = 32

MULTIPLIER OF PARTICLE NUMBER AT SOURCE = 1.00

SCHEME FOR CONCENTRATION INTERPOLATION IS [LINEAR]

PARTICLES FOR APPROXIMATING A SINK CELL IN THE [MMOC] SCHEME

ARE PLACED RANDOMLY WITHIN CELL BLOCK

NUMBER OF PARTICLES USED TO APPROXIMATE A SINK CELL IN THE

[MMOC] SCHEME = 16

CRITICAL CONCENTRATION GRADIENT USED IN THE "HMOC" SCHEME

[DCHMOC] = 0.1000E-02

THE "MOC" SOLUTION IS USED WHEN DCCELL > DCHMOC

THE "MMOC" SOLUTION IS USED WHEN DCCELL =< DCHMOC

DISPERSION PARAMETERS

---

LONG. DISPERSIVITY (AL) = 0.6000000 FOR LAYER 1

H. TRANS./LONG. DISP. = 0.1670000

V. TRANS./LONG. DISP. = 0.1670000

DIFFUSION COEFFICIENT = 0.000000

SORPTION AND 1ST ORDER RATE REACTION PARAMETERS

---

BULK DENSITY (RHOB) = 104.0000

SORPTION CONSTANT NO. 1 = 0.3000000E-02

SORPTION CONSTANT NO. 2 = 0.000000

RETARD. FACTOR IN LAYER 1 FOR TIME STEP 1, STRESS PERIOD 1

1	2	3	4	5	6	7	8	9	10	11
12	13	14	15	16	17	18	19	20	21	22
23	24	25	26	27	28	29	30	31	32	33
34	35	36	37	38	39	40	41	42	43	
<hr/>										
<b>1</b>	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
<b>2</b>	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
<b>3</b>	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95
<b>4</b>	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95	1.95













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STRESS PERIOD NO. 001

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LENGTH OF CURRENT STRESS PERIOD = 100.0000

NUMBER OF TIME STEPS FOR CURRENT STRESS PERIOD = 10

TIME STEP MULTIPLIER = 1.000000

USER-SPECIFIED TRANSPORT STEPSIZE = 0.000000 days

MAXIMUM NUMBER OF TRANSPORT STEPS ALLOWED IN ONE TIME STEP

= 1000

NO LAYER ROW COLUMN CONCENTRATION TYPE

1 1 19 3 0.5000000E-02 WELL

2 1 19 4 0.5000000E-02 WELL

3 1 19 5 0.5000000E-02 WELL

4 1 19 6 0.5000000E-02 WELL

5 1 19 7 0.5000000E-02 WELL

6 1 19 8 0.5000000E-02 WELL

7 1 19 9 0.5000000E-02 WELL

8 1 19 10 0.5000000E-02 WELL

9 1 19 11 0.5000000E-02 WELL

10 1 19 12 0.5000000E-02 WELL

11 1 19 13 0.5000000E-02 WELL

12 1 19 14 0.5000000E-02 WELL

13 1 19 15 0.5000000E-02 WELL

14 1 19 22 0.000000 WELL

CUMMULATIVE MASS BUDGETS AT END OF TRANSPORT STEP 1, TIME  
STEP 2, STRESS PERIOD 10

	IN	OUT
CONSTANT CONCENTRATION:	0.000000	0.000000
CONSTANT HEAD:	0.000000	-0.5297388E-08
WELLS:	49.77857	-14.51752
DECAY OR BIODEGRADATION:	0.000000	0.000000
MASS STORAGE (SOLUTE):	31.06653	-51.02594
MASS STORAGE (ADSORBED):	28.49554	-44.86256
[TOTAL]:	109.3406 mg	-110.4060 mg
NET (IN - OUT):	-1.065376	
DISCREPANCY (PERCENT):	-0.9696406	

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## *Vita*

Captain Tay William Johannes was born 2 March 1967 in Bozeman, Montana to the parents of James and Cheryl Johannes. He graduated from Wibaux County High School, Wibaux, Montana in 1985. He then attended Montana State University (MSU) from 1985 through 1990 and graduated with a Bachelor of Science Degree in Electrical Engineering. He was commissioned into the Air Force on 16 March 1990 and was assigned to March AFB, CA in September of 1990. At March AFB, he became an electrical design engineer for two and half years, before going overseas to Korea and then Japan. Captain Johannes departed Japan (Misawa AB) and entered the School of Engineering, Air Force Institute of Technology, in August of 1997. On 3 February 1994, he married the former, Miss Tae O. Kwon, and they currently have two children, Daniel age 3, and Jay age 8 months. He and his family are preparing to depart for Randolph AFB, TX, where he will be assigned to HQ/AETC to work in the Environmental Directorate.

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